Supporting Information

Mechanism and Enantioselectivity in Palladium-Catalyzed Conjugate Addition of Arylboronic Acids to β-Substituted Cyclic Enones: Insights from Computation and Experiment

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Contents

Complete Reference of Gaussian 03 (Ref. 29 in the manuscript)

Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, **2004**.

***Cis/trans* Isomerization of Cationic Phenylpalladium(II) Complexes**

Attempts to optimize the transition state of the isomerization of the tricooridnated cationic phenylpalladium(II) complexes **11** and **11'** failed. We then performed a scan of the reaction coordinates by calculating structures with fixed N-Pd-C angle. The results are summarized in Figure S1. Based on the scan of the reaction coordinate (i.e. N-Pd-C angle), we estimate the activation barrier for the isomerization of **11** to **11'** is higher than 10 kcal/mol with respect to **11**. Thus, the isomerization has higher activation energy than subsequent alkene insertion (**14-ts** is only 1.7 kcal/mol less stable than **11**).

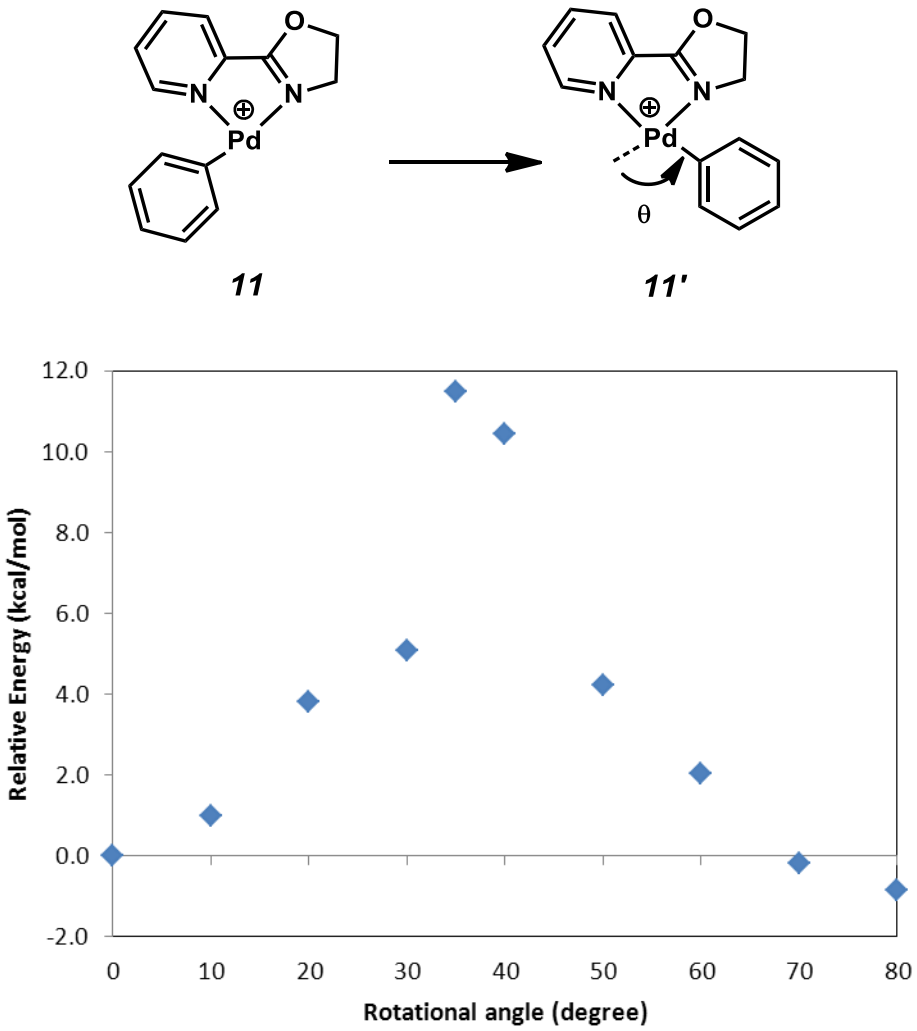
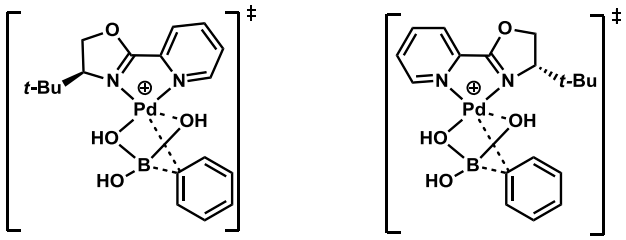


Figure S1. Scan of the reaction coordinate of the interconversion between **11** and **11'**. The energies in kcal/mol are calculated at the BP86/6-31G(d)-SDD level without solvent corrections

Selectivity of Formation of the *cis* and *trans* Products in Transmetalation

We attempted to compute the activation energies of transmetalation leading to cis and trans cationic phenylpalladium(II) complexes (**11** and **11'**) with the (*S*)-*t*-BuPyOx ligand. However, the geometry optimizations cannot locate the transmetalation transition states. We then performed a scan of the forming Pd–C(phenyl) bond in the *cis* and *trans* pathway (Table S1). In **s1-ts**, the phenyl is *trans* to the oxazoline on the ligand. In **s2-ts**, the phenyl is *cis* to oxazoline. We fixed the forming Ph-C bond distance in both structures to 2.20, 2.35, 2.40, 2.45, 2.50, 2.55 and 2.60 Å, respectively. In all distances, the *cis* structure **s2-ts** are at least 2.0 kcal/mol less stable than the *trans* isomer **s1-ts**. This indicates the formation of the *trans* product is favored in transmetalation. In the *cis* pathway, the phenyl is adjacent to the bulky *t*-Bu group on the ligand, and the transition state **s2-ts** is destabilized by the steric repulsions between *t*-Bu and Ph.

Table S1. Scan of the forming Pd–C(phenyl) bond in pathways **s1-ts** and **s2-ts**.[a]



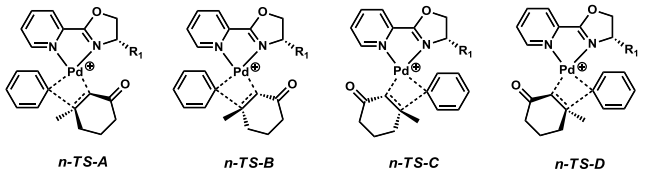
s1-ts *s2-ts*

R_{Pd-C}	E_{s1-ts}	E_{s2-ts}	ΔE
2.20	5.6	9.5	3.9
2.35	8.3	11.3	3.0
2.40	8.8	11.9	3.0
2.45	9.5	12.5	3.0
2.50	10.1	13.1	3.0
2.55	10.8	13.6	2.7
2.60	11.6	14.0	2.4

[a]The values are energies in kcal/mol calculated at the BP86/6-31G(d)-SDD level without solvent corrections

Activation Free Energies and Enantioselectivities for Table 4-7

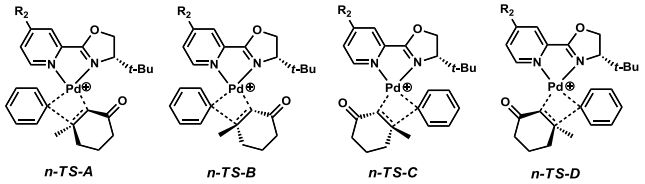
Table S2. Activation free energies and enantioselectivities of alkene insertion with (*S*)-*t*-BuPyOX, (*S*)-*i*-PrPyOX, (*S*)-*i*-BuPyOX, and (*S*)-PhPyOx ligands



TS	R^1	$\Delta G^{\ddagger}$ [a]				ee [b]
		TS-A	**TS-B**	**TS-C**	**TS-D**	
1	*t*-Bu	**23.2**	**26.0**	25.7	26.0	97% [93%]
2	*i*-Pr	**23.0**	24.6	24.4	**24.3**	76% [40%]
3	*i*-Bu	**22.5**	**23.6**	24.7	23.9	68% [24%]
4	Ph	**22.5**	**23.8**	23.8	24.4	74% [52%]

[a]The values are activation free energies in kcal/mol calculated at the BP86/6-31G(d)–SDD level and the CPCM solvation model in dichloroethane. Experimental ee are given in square brackets.

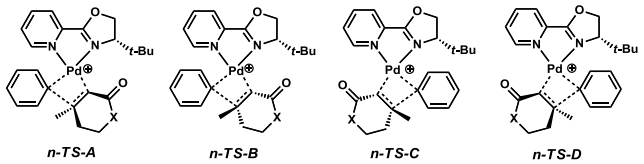
Table S3. Remote ligand substituent effects on activation free energies and enantioselectivities of alkene insertion.



TS	R^2	$\Delta G^{\ddagger}$ [a]				ee [b]
		TS-A	**TS-B**	**TS-C**	**TS-D**	
1	H	**23.2**	**26.0**	25.7	26.0	97% [93%]
5	CF_3	**23.6**	26.6	26.1	**26.4**	97% [81%]
6	OCH_3	**23.7**	**26.1**	25.7	26.5	95% [78%]

[a]The values are activation free energies in kcal/mol calculated at the BP86/6-31G(d)–SDD level and the CPCM solvation model in dichloroethane. Experimental ee are given in square brackets.

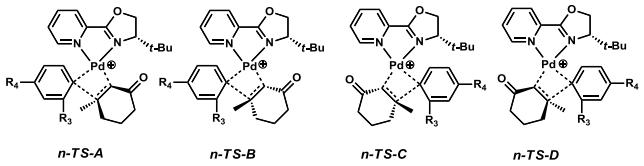
Table S4. Activation free energies and enantioselectivities of alkene insertion with substrates varying at the α'-position.[a]



TS	X	ΔG‡ [a]				ee [b]
		TS-A	**TS-B**	**TS-C**	**TS-D**	
1	CH_2	**23.2**	**26.0**	25.7	26.0	97% [93%]
7	O	**21.6**	**23.4**	23.7	23.9	87% [57%]
8	$C(CH_3)_2$	**22.2**	26.6	23.8	**25.1**	97% [90%]

[a]The values are activation free energies in kcal/mol calculated at the BP86/6-31G(d)–SDD level and the CPCM solvation model in dichloroethane. Experimental ee are given in square brackets.

Table S5. Activation free energies and enantioselectivities of alkene insertion with various boronic acids.[a]



TS	R^3	R^4	ΔG‡ [a]				ee [b]
			TS-A	**TS-B**	**TS-C**	**TS-D**	
1	H	H	**23.2**	**26.0**	25.7	26.0	97% [93%]
9	H	CH_3CO	**26.6**	**28.9**	29.1	29.4	94% [96%]
10	H	CF_3	**26.3**	**28.8**	27.9	28.8	96% [96%]

[a]The values are activation free energies in kcal/mol calculated at the BP86/6-31G(d)–SDD level and the CPCM solvation model in dichloroethane. Experimental ee are given in square brackets.

Computational Investigations on the Effects of Boronic Acid on Alkene Insertion

We investigated if coordination of phenylboronic acid will activate the enone in the alkene insertion step (**14-ts**, Figure 3). Two different binding modes between the alkene insertion transition state **14-ts** and phenylboronic acid are considered in the calculations (Figure S2): the boronic acid acting as a hydrogen bonding donor (**s3-ts-B**) and as a Lewis acid that the B atom is coordinated with the enone oxygen (**s3-ts-C**). **s3-ts-B** is 9.1 kcal/mol less stable than the uncoordinated **14-ts** in terms of Gibbs free energy. The structure of **s3-ts-B** is shown in Figure S3. Geometry optimization of **s3-ts-C** was not successful and always leading to dissociation of the B–O bond, indicating the interaction between B and O is not stabilizing.

These results suggest that binding with boronic acid does not accelerate the alkene insertion.

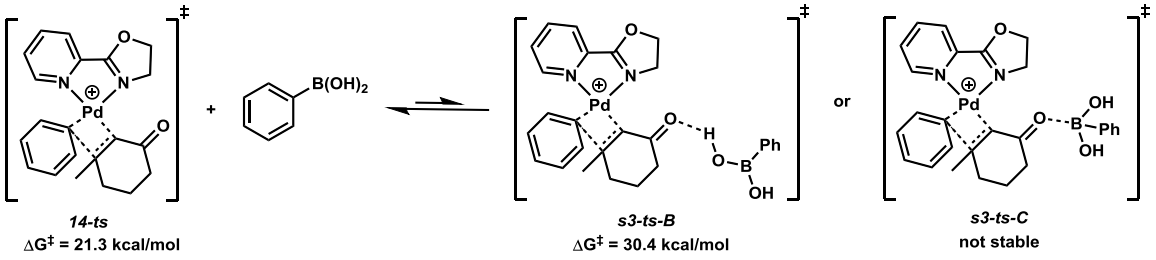


Figure S2. Activation free energies of alkene insertion with boronic acid coordination. Energies are with respect to the Pd(PyOx)Ph–enone complex **12**.

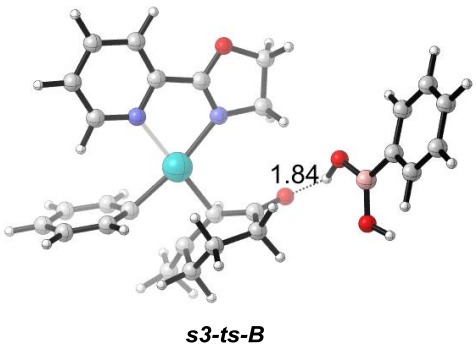


Figure S3. Optimized structure of the alkene insertion transition state coordinated with phenylbornic acid (**s3-ts-B**).

Computed Potential Energy Surface of the Catalytic Cycle with *t*-Bu-PyOx Ligand

We have calculated the catalytic cycle in Figure 3 with the model ligand replaced with the *t*-Bu-PyOx ligand, and the results are in Figure S4. As mentioned above, the transmetalation transition state, **7-ts**, was not located. According to the scan of Pd-C bond length in Figure S5, the barrier is estimated to be around 11 kcal/mol.

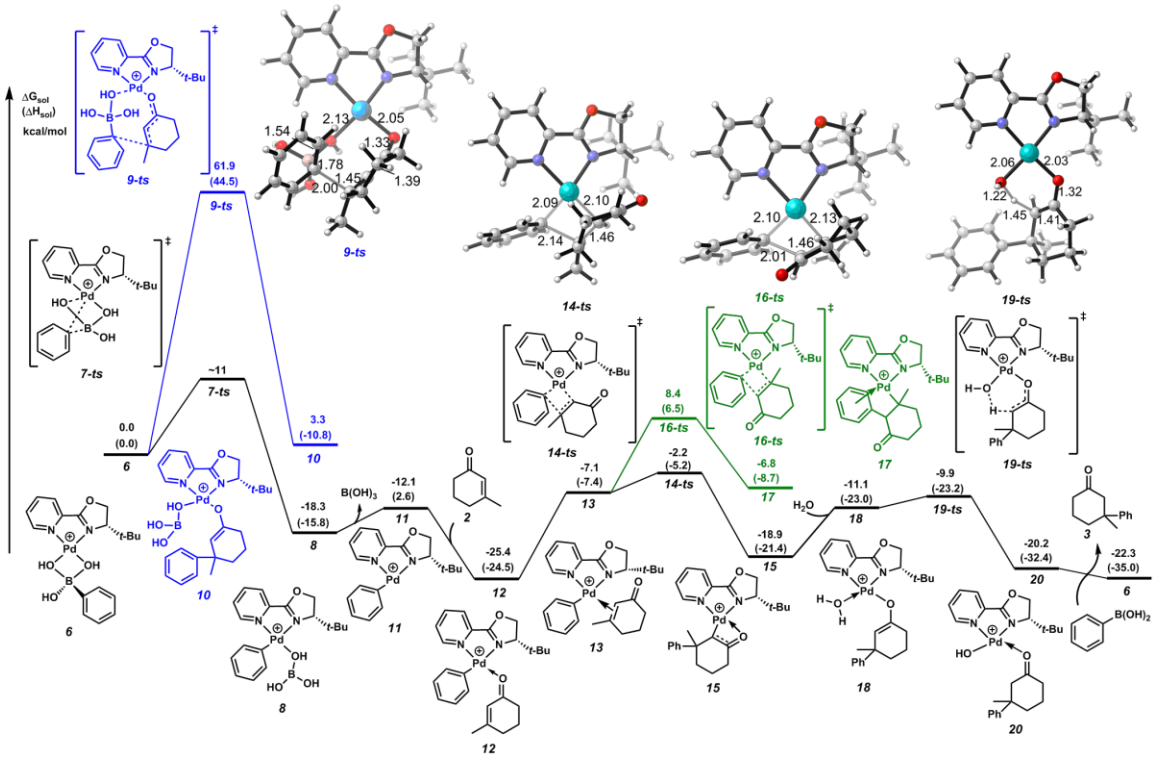


Figure S4. Computed potential energy surface of the catalytic cycle with *t*-Bu-PyOx ligand (shown in black), the alternative direct nucleophilic addition pathway (via **9-ts**, shown in blue), and the regioisomeric carbopalladation pathway (via **16-ts**, shown in green).

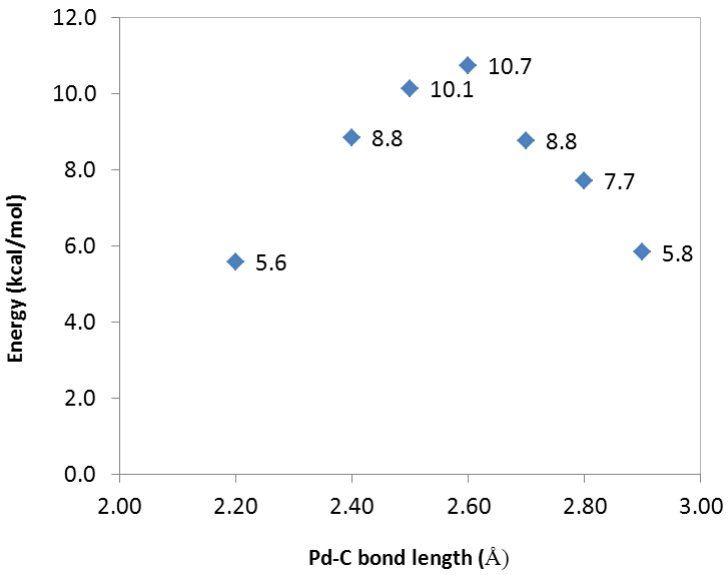


Figure S5. Scan of the reaction coordinate of the Pd-C bond length in the transmetalation process**.** The energies are calculated at the BP86/6-31G(d)-SDD level without solvent corrections

The Cartesian Coordinates (Å) for Complexes and Transition State Geometries

Numbering correspond to the items in Table S2-S5. Energies in solvation, E(Solv), and thermal corrections to enthalpy (H) and Gibbs free energies (G) at 298K are included.

Complex 12 for TS1

E(Solv): -1359.135474

Correction to H: 0.532059

Correction to G: 0.437003

C	-2.76545	-0.48736	-0.73206
C	-3.15809	-2.62102	-1.27494
C	-1.87518	-2.52639	-0.39431
N	-1.67646	-1.05257	-0.29709
H	-3.92877	-3.30317	-0.88972
C	-2.96827	0.96365	-0.64250
C	-4.17626	1.58831	-0.97368
N	-1.88438	1.65451	-0.15993
C	-4.29602	2.97310	-0.78216
H	-4.99964	0.98427	-1.36410
C	-2.01231	2.98867	0.02922
C	-3.19985	3.67592	-0.26588
H	-5.22978	3.48827	-1.02706
H	-1.12831	3.50127	0.41415
H	-3.24703	4.75418	-0.08858
Pd	-0.19717	0.50367	0.17232
C	3.54316	-1.69329	0.37338
C	2.46579	-0.88675	-0.16162
C	2.61699	-0.25560	-1.52568
C	3.59729	-1.03557	-2.41913
C	4.92382	-1.29780	-1.68551
C	4.72194	-1.87551	-0.30283
H	1.61403	-0.15696	-1.98092
H	3.39878	-2.10363	1.37915
H	3.14406	-2.00492	-2.70115
H	3.77917	-0.48087	-3.35550
H	5.57499	-1.96830	-2.27677
H	5.49809	-0.35179	-1.57669
H	2.97550	0.78183	-1.35654
O	1.43580	-0.70983	0.56245
C	5.86851	-2.62649	0.30732
H	5.66837	-2.93555	1.34549
H	6.09895	-3.52811	-0.29342
H	6.78719	-2.00865	0.29189
C	0.99242	2.07190	0.52530
C	1.57524	2.20912	1.80135
C	1.26394	3.03374	-0.47136
C	2.40641	3.31088	2.08199
H	1.38468	1.46393	2.58264
C	2.10627	4.12716	-0.18602
H	0.82339	2.94154	-1.47201
C	2.67444	4.26859	1.09024
H	2.84415	3.41526	3.08153
H	2.31468	4.86698	-0.96788

H	3.32417	5.12228	1.31112	H	-4.01430	0.08134	-2.10633
O	-3.73557	-1.26306	-1.24546	H	-2.93202	-1.50331	-0.62949
H	-1.00667	-2.96086	-0.92150	C	-0.96377	2.47057	-0.65250
H	-2.94905	-2.85581	-2.33186	C	-1.22051	3.80419	-0.99501
C	-1.98644	-3.22434	1.00624	N	0.25819	2.03419	-0.22401
C	-0.67533	-3.00964	1.79235	C	-0.17992	4.73760	-0.86833
H	0.19683	-3.39811	1.23534	H	-2.21653	4.09107	-1.34273
H	-0.49439	-1.94247	2.00399	C	1.24926	2.93972	-0.09989
H	-0.72341	-3.54565	2.75714	C	1.06771	4.29934	-0.40516
C	-2.17711	-4.74094	0.76455	H	-0.34554	5.78897	-1.12288
H	-2.19360	-5.27329	1.73168	H	2.21006	2.55445	0.25063
H	-3.12605	-4.97822	0.24982	H	1.90291	4.99431	-0.27927
H	-1.34842	-5.16305	0.16606	Pd	0.34791	-0.13103	0.03202
C	-3.17165	-2.66201	1.82118	C	0.46258	-2.22042	0.15049
H	-3.03831	-1.58694	2.03869	C	-0.35369	-2.72242	-1.01218
H	-4.14230	-2.79565	1.30913	C	0.30021	-2.78950	-2.38966
H	-3.24303	-3.18695	2.78984	C	1.65735	-2.07347	-2.45642
				C	2.53775	-2.50898	-1.27733

1-TS-A

E(Solv):	-1359.103397			C	1.91715	-2.22540	0.08621
Correction to H:	0.530607			H	0.01431	-2.48036	1.12220
Correction to G:	0.441858			O	-1.50871	-3.12232	-0.82805
C	-1.99027	1.42110	-0.66353	C	2.66712	-2.83839	1.25809
C	-3.94407	0.41237	-1.05634	H	2.21797	-2.58185	2.22957
C	-3.05598	-0.50596	-0.17647	H	2.60229	-3.93957	1.14602
N	-1.74396	0.20909	-0.24373	H	3.73265	-2.55842	1.26276
				C	2.38949	-0.17440	0.45879

C	2.59240	0.08732	1.84008	H	2.16251	-2.29417	-3.41308
C	3.34606	0.30734	-0.46887	H	3.55905	-2.09745	-1.33271
C	3.70102	0.83127	2.27350	H	2.66132	-3.61372	-1.31484
H	1.87986	-0.28811	2.58401	H	0.42408	-3.86690	-2.62208
C	4.47187	1.02389	-0.02883	H	-0.41799	-2.40386	-3.13526
H	3.21401	0.13489	-1.54206				
C	4.65112	1.28778	1.34120	**1-TS-B**			
H	3.83392	1.03621	3.34144	E(Solv):	-1359.099789		
H	5.20755	1.37867	-0.75927	Correction to H:	0.530647		
H	5.53273	1.84053	1.68285	Correction to G:	0.442730		
O	-3.23372	1.71189	-1.06938	C	-1.82515	1.65448	-0.58432
H	-4.94932	0.60416	-0.65737	C	-3.68619	0.85750	-1.52110
C	-3.57414	-0.69726	1.29478	C	-3.03541	-0.24190	-0.64808
C	-2.54551	-1.51422	2.10664	N	-1.69283	0.36942	-0.38245
H	-1.59884	-0.95630	2.22690	H	-4.75179	1.03626	-1.32639
H	-2.94327	-1.72402	3.11559	C	-0.78817	2.61333	-0.18055
H	-2.32687	-2.47607	1.61091	C	-0.95905	4.00288	-0.22095
C	-3.82366	0.65471	1.99944	N	0.34554	2.01723	0.29517
H	-2.89632	1.25066	2.08504	C	0.07130	4.81478	0.27901
H	-4.58573	1.26979	1.48729	H	-1.88273	4.42365	-0.62723
H	-4.19059	0.47716	3.02572	C	1.33240	2.80524	0.76611
C	-4.89253	-1.50468	1.21711	C	1.22663	4.20630	0.78795
H	-4.73768	-2.48200	0.72574	H	-0.03080	5.90436	0.27197
H	-5.27294	-1.69659	2.23581	H	2.22435	2.28905	1.13258
H	-5.69040	-0.96842	0.67153	H	2.04845	4.80135	1.19646
H	1.49675	-0.97607	-2.42063	Pd	0.38454	-0.11781	-0.15446

C	0.50515	-2.02259	-1.01218	C	-3.83323	-0.54971	0.67525
C	-0.51761	-2.92578	-0.38054	C	-5.16440	-1.22491	0.26380
C	-0.13096	-3.67975	0.88722	H	-5.82658	-0.55307	-0.31218
C	1.15040	-3.14002	1.53811	H	-5.72220	-1.52870	1.16700
C	2.27062	-3.05040	0.49306	H	-4.98422	-2.13219	-0.34065
C	1.92261	-2.16807	-0.70240	C	-3.03934	-1.53714	1.55610
H	0.25812	-1.80395	-2.06599	H	-2.04892	-1.12857	1.82884
O	-1.61231	-3.08870	-0.93073	H	-2.89553	-2.49608	1.03113
C	2.87297	-2.30875	-1.88184	H	-3.59375	-1.73338	2.49114
H	2.61869	-1.63554	-2.71482	C	-4.12267	0.73189	1.48922
H	2.76828	-3.34604	-2.25863	H	-4.71148	1.47671	0.92449
H	3.92486	-2.15516	-1.59302	H	-3.19166	1.21580	1.83762
C	2.46816	-0.21535	-0.06094	H	-4.70771	0.47251	2.38911
C	3.09556	0.52271	-1.09891	H	2.43719	-4.06413	0.06735
C	3.06712	-0.21474	1.22471	H	3.23779	-2.75061	0.92886
C	4.27536	1.24271	-0.85727	H	0.94682	-2.13840	1.96824
H	2.65808	0.53815	-2.10347	H	1.46169	-3.79074	2.37392
C	4.25564	0.49743	1.46121	H	0.00731	-4.73992	0.59105
H	2.60888	-0.76814	2.05091	H	-0.99074	-3.67030	1.57929
C	4.86478	1.22169	0.42037				
H	4.74246	1.80913	-1.67045	**1-TS-C**			
H	4.70766	0.48021	2.45917	E(Solv):	-1359.099333		
H	5.79923	1.76311	0.60268	Correction to H:	0.530596		
O	-2.96549	2.09500	-1.13383	Correction to G:	0.441836		
H	-3.51751	0.72036	-2.60310	C	-2.28601	0.82065	-0.54475
H	-2.88884	-1.18416	-1.20148	C	-3.66313	-0.90688	-0.87233

C	-2.45201	-1.36076	-0.01389	H	3.89373	-1.90404	-1.64710
N	-1.55057	-0.17591	-0.13446	C	1.20923	-1.51384	-0.74455
H	-3.61239	-1.24995	-1.91965	C	1.01261	-1.62015	-2.14630
H	-1.94730	-2.23377	-0.46198	C	1.09175	-2.67658	0.04932
C	-1.76977	2.19295	-0.60167	C	0.66976	-2.85030	-2.72801
C	-2.55967	3.29066	-0.96301	H	1.12854	-0.73932	-2.78908
N	-0.45174	2.30625	-0.24541	C	0.77265	-3.91223	-0.54005
C	-1.97766	4.56810	-0.94946	H	1.24069	-2.62796	1.13223
H	-3.60437	3.13316	-1.24442	C	0.55764	-4.00119	-1.92626
C	0.10167	3.53787	-0.24307	H	0.51339	-2.91438	-3.81055
C	-0.63249	4.68885	-0.58126	H	0.69410	-4.80688	0.08791
H	-2.56785	5.44845	-1.22223	H	0.31848	-4.96716	-2.38366
H	1.15750	3.58985	0.05319	O	-3.55502	0.56761	-0.90212
H	-0.13580	5.66293	-0.55052	H	-4.64759	-1.14566	-0.44809
Pd	0.53370	0.36920	-0.14242	C	-2.81814	-1.69920	1.47780
C	2.55470	0.94198	-0.18584	C	-1.53559	-2.01013	2.27733
C	2.75460	1.72448	1.08500	H	-0.84513	-1.14781	2.28552
C	3.04114	0.97042	2.37886	H	-1.79266	-2.25058	3.32430
C	2.81288	-0.54333	2.26330	H	-1.00410	-2.87905	1.85229
C	3.50774	-1.08365	1.00709	C	-3.56671	-0.53172	2.15985
C	3.03189	-0.42834	-0.28225	H	-2.94469	0.38046	2.20793
H	2.66712	1.56432	-1.08925	H	-4.51561	-0.27879	1.65420
O	2.74567	2.96200	1.05640	H	-3.81872	-0.80900	3.19844
C	3.82332	-0.81217	-1.51964	C	-3.71089	-2.96379	1.46819
H	3.41846	-0.36249	-2.43906	H	-3.20296	-3.81413	0.97701
H	4.85054	-0.41652	-1.38453	H	-3.94139	-3.26581	2.50483

H	-4.67750	-2.80183	0.95780
H	3.19036	-1.05986	3.16303
H	1.72387	-0.74690	2.20568
H	3.44941	-2.18153	0.92650
H	4.59324	-0.84805	1.07016
H	2.44230	1.42847	3.18609
H	4.10003	1.18103	2.63289

1-TS-D

E(Solv): -1359.098353

Correction to H: 0.530307

Correction to G: 0.441242

C	1.52760	1.77678	0.64002
C	3.19750	0.94593	1.86588
C	2.70369	-0.12438	0.85864
N	1.44570	0.50619	0.34946
H	4.28038	1.12819	1.85313
C	0.57769	2.75768	0.10258
C	0.80324	4.13868	0.14288
N	-0.50703	2.19611	-0.51446
C	-0.09973	4.98299	-0.52285
H	1.67761	4.52739	0.67171
C	-1.36465	3.01578	-1.15854
C	-1.18591	4.40984	-1.19476
H	0.04994	6.06707	-0.51870
H	-2.24105	2.54372	-1.61104
H	-1.91004	5.02452	-1.73686
Pd	-0.59147	0.04116	-0.28197
C	-2.63223	-0.33904	-0.63148
C	-3.37046	0.74747	0.10577
C	-3.52666	0.62691	1.61981
C	-2.71460	-0.53063	2.22096
C	-2.96332	-1.80881	1.41158
C	-2.59628	-1.68087	-0.06312
H	-2.78108	-0.27555	-1.72286
O	-3.87243	1.68344	-0.52577
C	-3.09049	-2.83518	-0.92024
H	-2.79945	-2.73894	-1.97652
H	-4.19857	-2.81754	-0.87977
H	-2.75282	-3.81098	-0.53497
C	-0.50084	-2.03600	-0.16878
C	-0.21022	-2.63522	-1.42268
C	-0.04080	-2.67424	1.01101
C	0.50864	-3.83738	-1.49340
H	-0.56465	-2.16785	-2.34893
C	0.67379	-3.88001	0.93819
H	-0.24838	-2.23478	1.99338
C	0.93764	-4.46965	-0.31249
H	0.72185	-4.28818	-2.46874
H	1.01427	-4.36720	1.85875
H	1.47279	-5.42381	-0.36550
O	2.54450	2.19181	1.41322

H	2.85939	0.76819	2.90133
H	2.44452	-1.06903	1.36664
C	3.73450	-0.44248	-0.28424
C	4.94336	-1.15942	0.36435
H	5.47848	-0.52430	1.09384
H	5.67321	-1.43838	-0.41570
H	4.63442	-2.08714	0.88048
C	3.09149	-1.38939	-1.31587
H	2.22932	-0.91714	-1.81695
H	2.74386	-2.32371	-0.84294
H	3.83059	-1.65728	-2.09202
C	4.20766	0.83950	-1.00567
H	4.72160	1.54924	-0.33280
H	3.36713	1.36649	-1.49271
H	4.92578	0.57110	-1.80022
H	-1.63292	-0.27849	2.19562
H	-2.98759	-0.68534	3.27951
H	-4.05286	-2.03083	1.42482
H	-2.47943	-2.69595	1.85245
H	-3.27159	1.60223	2.07216
H	-4.60809	0.47956	1.81428

Complex 12 for TS2

E(Solv): -1319.828941

Correction to H: 0.503562

Correction to G: 0.409803

C	-2.78760	-0.99171	-0.56656
C	-2.93764	-3.21605	-0.82583
C	-1.50470	-2.82923	-0.33876
N	-1.56071	-1.34667	-0.32384
H	-3.47253	-3.90239	-0.15213
C	-3.19315	0.41810	-0.51939
C	-4.50589	0.84606	-0.74662
N	-2.17446	1.28459	-0.20316
C	-4.80003	2.21365	-0.63755
H	-5.27169	0.10721	-0.99774
C	-2.46993	2.60047	-0.09429
C	-3.76577	3.09736	-0.30402
H	-5.81807	2.57729	-0.80677
H	-1.63264	3.25465	0.15989
H	-3.94543	4.17135	-0.20128
Pd	-0.32634	0.38907	0.09448
C	3.62074	-1.39465	0.42610
C	2.50374	-0.66433	-0.13565
C	2.67951	0.06954	-1.44368
C	3.78470	-0.55642	-2.31250
C	5.08255	-0.74103	-1.50774
C	4.85212	-1.42080	-0.17683
H	1.70332	0.10609	-1.96124
H	3.45509	-1.88258	1.39329
H	3.44591	-1.54320	-2.68126
H	3.96885	0.07266	-3.20009

H	5.83018	-1.31036	-2.09090	H	-0.19109	-5.21509	0.15400
H	5.55616	0.24469	-1.30634	C	-2.04310	-3.01119	2.18125
H	2.92586	1.12180	-1.18864	H	-2.13141	-1.91506	2.28236
O	1.41356	-0.64342	0.52021	H	-3.05700	-3.42982	2.03794
C	6.02655	-2.09729	0.46645	H	-1.66765	-3.40332	3.14221
H	5.79138	-2.49615	1.46593	H	-0.09659	-2.95396	1.25855
H	6.38729	-2.92745	-0.17181				
H	6.87617	-1.39297	0.55682	**2-TS-A**			
C	0.63826	2.10210	0.46676	E(Solv):	-1319.797871		
C	1.17300	2.31749	1.75341	Correction to H:	0.502212		
C	0.80107	3.09256	-0.52644	Correction to G:	0.415354		
C	1.84737	3.51876	2.04640	C	-2.12056	1.45270	-0.49967
H	1.06546	1.55605	2.53509	C	-4.13779	0.49256	-0.67630
C	1.48601	4.28778	-0.22861	C	-3.11962	-0.53240	-0.10211
H	0.39987	2.94259	-1.53696	N	-1.83207	0.21005	-0.22589
C	2.00620	4.50343	1.05766	H	-4.44580	0.27820	-1.71262
H	2.24779	3.68054	3.05395	H	-3.06279	-1.43668	-0.72932
H	1.61069	5.04770	-1.00908	C	-1.08795	2.49456	-0.54754
H	2.53357	5.43527	1.28845	C	-1.36398	3.84219	-0.81032
O	-3.69422	-1.94652	-0.83431	N	0.16956	2.02943	-0.28279
H	-0.74750	-3.13747	-1.08290	C	-0.30068	4.75803	-0.78766
H	-2.96437	-3.61025	-1.85385	H	-2.39076	4.15249	-1.02178
C	-1.08495	-3.40481	1.04300	C	1.18323	2.91832	-0.25938
C	-0.90893	-4.93300	0.94574	C	0.98831	4.28834	-0.50374
H	-0.53250	-5.33703	1.90112	H	-0.47983	5.81923	-0.98606
H	-1.86664	-5.44458	0.73327	H	2.17432	2.51175	-0.04199

H	1.84534	4.96708	-0.46901	H	-5.02675	0.64845	-0.04797
Pd	0.24937	-0.13484	0.01829	C	-3.38673	-0.98450	1.36040
C	0.32274	-2.20753	0.29904	C	-3.47513	0.18232	2.36051
C	-0.52287	-2.79605	-0.80080	H	-2.55431	0.79312	2.37242
C	0.10368	-2.98682	-2.17918	H	-4.32959	0.85091	2.14479
C	1.46741	-2.29552	-2.32832	H	-3.62444	-0.20711	3.38253
C	2.36530	-2.64756	-1.13461	C	-4.64386	-1.87528	1.40396
C	1.77607	-2.24396	0.21305	H	-4.54486	-2.74133	0.72681
H	-0.11417	-2.37684	1.29747	H	-4.80296	-2.26012	2.42588
O	-1.67893	-3.15774	-0.55943	H	-5.55692	-1.31701	1.12273
C	2.53606	-2.77951	1.41604	H	1.31994	-1.19652	-2.37671
H	2.11342	-2.43618	2.37240	H	1.95089	-2.59804	-3.27363
H	2.44393	-3.88419	1.39377	H	3.39066	-2.25714	-1.24254
H	3.60756	-2.52628	1.37780	H	2.47272	-3.75339	-1.08452
C	2.29783	-0.17997	0.41675	H	0.21102	-4.08105	-2.32444
C	2.54287	0.18169	1.76790	H	-0.62375	-2.65397	-2.94110
C	3.23652	0.21075	-0.56995	H	-2.52104	-1.61824	1.63074
C	3.67717	0.93258	2.11444				
H	1.84299	-0.12216	2.55532	**2-TS-B**			
C	4.38621	0.93721	-0.21584	E(Solv):	-1319.796152		
H	3.07295	-0.04329	-1.62246	Correction to H:	0.502206		
C	4.60857	1.29879	1.12525	Correction to G:	0.416169		
H	3.84393	1.21423	3.15991	C	-1.93292	1.71723	-0.45249
H	5.10753	1.22155	-0.99012	C	-3.91091	0.98743	-1.20116
H	5.50936	1.85764	1.40051	C	-3.09054	-0.20481	-0.64743
O	-3.40339	1.77716	-0.70944	N	-1.75274	0.42438	-0.44096

H	-4.92153	1.08211	-0.77928	C	2.97450	-0.22796	1.18518
C	-0.85743	2.64911	-0.09344	C	4.24817	0.93731	-1.03712
C	-1.02385	4.03854	-0.03787	H	2.58460	0.20382	-2.20367
N	0.32068	2.02708	0.21245	C	4.20753	0.42748	1.34458
C	0.06632	4.82495	0.36611	H	2.48714	-0.66217	2.06453
H	-1.98864	4.47904	-0.30345	C	4.84774	1.00743	0.23412
C	1.36285	2.79199	0.59477	H	4.74063	1.39115	-1.90416
C	1.27261	4.19100	0.69181	H	4.66826	0.48171	2.33723
H	-0.02851	5.91358	0.42530	H	5.81493	1.50630	0.35747
H	2.28747	2.25877	0.83166	O	-3.14821	2.18420	-0.77279
H	2.14540	4.76426	1.01733	H	-3.95748	1.01982	-2.30256
Pd	0.29130	-0.11959	-0.21809	H	-2.98920	-1.01685	-1.38515
C	0.32742	-2.08530	-0.93539	C	-3.63790	-0.80953	0.67869
C	-0.80115	-2.83966	-0.28571	C	-4.89263	-1.65334	0.38115
C	-0.56543	-3.43541	1.10022	H	-5.71591	-1.03897	-0.03015
C	0.71519	-2.91296	1.76839	H	-5.26926	-2.11871	1.30832
C	1.89898	-3.05321	0.80216	H	-4.66648	-2.45960	-0.33752
C	1.70479	-2.30296	-0.51222	C	-3.89287	0.23475	1.78091
H	0.16354	-1.95507	-2.01926	H	-4.69938	0.94125	1.51112
O	-1.85891	-3.00951	-0.90022	H	-2.98584	0.81908	2.02014
C	2.71936	-2.65398	-1.58946	H	-4.20924	-0.27153	2.70931
H	2.58119	-2.06673	-2.50986	H	1.99775	-4.12324	0.51588
H	2.55781	-3.71882	-1.85244	H	2.86258	-2.78255	1.26413
H	3.75696	-2.54324	-1.23611	H	0.57811	-1.84733	2.04678
C	2.36497	-0.32018	-0.09150	H	0.91637	-3.46682	2.70204
C	3.02653	0.26681	-1.20242	H	-0.50351	-4.53433	0.96278

H	-1.46518	-3.26316	1.71736
H	-2.84915	-1.49668	1.03657

2-TS-C

E(Solv): -1319.795403

Correction to H: 0.502125

Correction to G: 0.415116

C	2.31884	1.05433	-0.32939
C	2.20418	3.28920	-0.43653
C	0.83608	2.71385	0.03307
N	1.04539	1.25073	-0.13713
H	2.18926	3.67840	-1.46784
H	0.01925	3.02915	-0.63923
C	2.87819	-0.29712	-0.43312
C	4.23776	-0.54594	-0.65280
N	1.94707	-1.29421	-0.30248
C	4.66888	-1.87868	-0.74674
H	4.93004	0.29485	-0.74925
C	2.37010	-2.57246	-0.40304
C	3.72041	-2.90028	-0.62146
H	5.72527	-2.10860	-0.91666
H	1.60222	-3.34668	-0.27984
H	4.00598	-3.95412	-0.68693
Pd	-0.09736	-0.54912	-0.21399
C	-1.22402	-2.32015	-0.31338
C	-0.77895	-3.15224	0.85838
C	-1.39124	-2.88304	2.22927
C	-2.21276	-1.58731	2.28341
C	-3.18263	-1.53674	1.09550
C	-2.49051	-1.60411	-0.26078
H	-0.96040	-2.77974	-1.28086
O	0.02956	-4.07420	0.68910
C	-3.43390	-1.76321	-1.44134
H	-2.90718	-1.76594	-2.40762
H	-3.92709	-2.75039	-1.33274
H	-4.21769	-0.98937	-1.45389
C	-1.89401	0.42961	-0.62524
C	-1.92799	0.74781	-2.00862
C	-2.49788	1.32202	0.29116
C	-2.52538	1.93637	-2.45516
H	-1.48764	0.06452	-2.74448
C	-3.11694	2.49959	-0.16178
H	-2.49150	1.10577	1.36446
C	-3.13094	2.80976	-1.53307
H	-2.53702	2.16948	-3.52561
H	-3.59072	3.17386	0.56031
H	-3.62360	3.72270	-1.88424
O	3.11818	2.12725	-0.43288
H	2.63835	4.04081	0.23870
C	0.44339	3.07359	1.49422
C	1.50882	2.67508	2.53103
H	1.73541	1.59469	2.49365

H	2.45438	3.23228	2.39547
H	1.14733	2.90128	3.54905
C	0.08188	4.56876	1.58682
H	-0.71701	4.83961	0.87314
H	-0.27269	4.81572	2.60220
H	0.95403	5.21779	1.38277
H	-2.76849	-1.52277	3.23522
H	-1.52673	-0.71580	2.24921
H	-3.86784	-0.67425	1.13834
H	-3.83625	-2.43609	1.13261
H	-0.58068	-2.90227	2.97945
H	-2.03553	-3.75582	2.45970
H	-0.47243	2.48838	1.70361

2-TS-D

E(Solv): -1319.795653

Correction to H: 0.502156

Correction to G: 0.415219

C	0.23991	2.48254	0.54071
C	2.18379	2.94576	1.55437
C	2.24455	1.52473	0.92087
N	0.84286	1.33018	0.45505
H	2.98454	3.62333	1.22435
C	-1.12665	2.67539	0.04463
C	-1.74061	3.93087	-0.03211
N	-1.73039	1.52127	-0.37804
C	-3.02315	4.01608	-0.59678
H	-1.21033	4.81322	0.33619
C	-2.96176	1.61455	-0.92419
C	-3.63362	2.84289	-1.05512
H	-3.53024	4.98262	-0.67641
H	-3.43462	0.67141	-1.21840
H	-4.63028	2.85709	-1.50537
Pd	-0.47545	-0.24135	-0.18414
C	-1.81988	-1.79915	-0.63046
C	-3.02672	-1.53496	0.22896
C	-2.98558	-1.94149	1.69984
C	-1.59335	-2.38840	2.17085
C	-1.00327	-3.39029	1.17074
C	-0.87919	-2.84232	-0.24656
H	-2.04490	-1.71622	-1.70732
O	-4.04430	-1.04515	-0.27547
C	-0.52714	-3.89208	-1.28809
H	-0.41037	-3.46894	-2.29686
H	-1.37504	-4.60568	-1.32642
H	0.38026	-4.45659	-1.01969
C	0.95781	-1.74969	-0.24382
C	1.56384	-1.82511	-1.52571
C	1.74166	-2.05217	0.89640
C	2.91235	-2.18982	-1.66037
H	0.97729	-1.60690	-2.42601
C	3.08733	-2.42904	0.75785

H	1.30370	-1.99554	1.89891
C	3.67215	-2.50642	-0.51948
H	3.36474	-2.24304	-2.65672
H	3.67787	-2.67063	1.64870
H	4.71620	-2.81972	-0.62571
O	0.90951	3.51635	1.07324
H	2.13291	2.93798	2.65540
H	2.46596	0.76155	1.68741
C	3.26916	1.36683	-0.23624
C	4.70483	1.44093	0.31966
H	4.94079	2.44048	0.73099
H	5.43534	1.24350	-0.48356
H	4.87279	0.69602	1.11832
C	3.04992	2.36733	-1.38528
H	3.21310	3.41436	-1.06771
H	2.03384	2.28927	-1.81119
H	3.76601	2.16621	-2.20073
H	-0.92781	-1.50407	2.25557
H	-1.65456	-2.84155	3.17584
H	-1.69400	-4.25798	1.08776
H	-0.04183	-3.81293	1.50678
H	-3.38568	-1.10487	2.30030
H	-3.71418	-2.76919	1.81526
H	3.11175	0.34737	-0.63444

Complex 12 for TS3

E(Solv): -1359.138192

Correction to H: 0.532739

Correction to G: 0.435295

C	2.72879	1.09435	-0.59399
C	2.59562	3.30520	-0.96488
C	1.21155	2.75751	-0.48915
N	1.46064	1.29614	-0.39044
H	3.01594	4.07954	-0.30406
C	3.31567	-0.24452	-0.46299
C	4.67850	-0.50518	-0.64567
N	2.41330	-1.22082	-0.11566
C	5.14822	-1.81357	-0.45622
H	5.34538	0.31489	-0.92521
C	2.87796	-2.47770	0.07188
C	4.23252	-2.80788	-0.08938
H	6.20894	-2.04688	-0.58925
H	2.13011	-3.22331	0.35078
H	4.55025	-3.84124	0.07650
Pd	0.45685	-0.56663	0.10685
C	-3.70751	0.64743	0.32519
C	-2.48535	0.07806	-0.20309
C	-2.52860	-0.70202	-1.49570
C	-3.70147	-0.26968	-2.39325
C	-5.02441	-0.26436	-1.60783
C	-4.91915	0.47393	-0.29281
H	-1.54977	-0.60300	-2.00038

H	-3.63247	1.17519	1.28263	C	0.33614	4.81902	0.84027
H	-3.50929	0.74782	-2.78347	H	1.18591	5.40253	0.42558
H	-3.77579	-0.94030	-3.26629	H	-0.12990	2.71856	1.20227
H	-5.84104	0.17035	-2.21390	H	1.54160	3.16297	1.60627
H	-5.34516	-1.30598	-1.38684	C	-0.90000	5.08485	-0.04110
H	-2.61914	-1.77321	-1.21767	H	-1.77571	4.52113	0.33269
O	-1.41604	0.23048	0.46882	H	-1.16396	6.15687	-0.02747
C	-6.19180	0.98018	0.31980	H	-0.74241	4.80296	-1.09844
H	-6.03505	1.42994	1.31309	C	0.09422	5.31307	2.28002
H	-6.66174	1.73408	-0.34164	H	0.98913	5.17516	2.91292
H	-6.92780	0.15843	0.41432	H	-0.16624	6.38589	2.29029
C	-0.27132	-2.37777	0.54461	H	-0.74036	4.76065	2.75133
C	-0.77389	-2.61982	1.83925				
C	-0.29607	-3.41366	-0.41457	**3-TS-A**			
C	-1.27767	-3.89162	2.17489	E(Solv):	-1359.107185		
H	-0.77292	-1.82423	2.59379	Correction to H:	0.531249		
C	-0.81111	-4.68070	-0.07418	Correction to G:	0.440116		
H	0.08217	-3.24384	-1.43072	C	-1.38003	2.10881	-0.56670
C	-1.29819	-4.92184	1.22058	C	-3.56447	1.75362	-0.91237
H	-1.65417	-4.07220	3.18844	C	-2.90692	0.45829	-0.36335
H	-0.82932	-5.47666	-0.82800	N	-1.45658	0.81685	-0.40080
H	-1.69278	-5.90892	1.48458	H	-3.82572	1.69972	-1.98232
O	3.50883	2.14504	-0.90029	H	-3.07234	-0.40252	-1.02938
H	0.43735	2.92200	-1.25908	C	-0.10258	2.82581	-0.47904
H	2.60343	3.66077	-2.00737	C	0.01685	4.21132	-0.64455
C	0.73400	3.32231	0.86391	N	0.96017	2.01558	-0.19232

C	1.28523	4.79423	-0.49825	H	3.37392	-0.70866	-1.37735
H	-0.87010	4.80643	-0.87806	C	4.82611	0.02179	1.63443
C	2.17355	2.58596	-0.05156	H	3.80113	0.04192	3.55293
C	2.37613	3.96921	-0.19452	H	5.56610	-0.08006	-0.40813
H	1.41513	5.87421	-0.61816	H	5.79674	0.30049	2.05828
H	2.99791	1.90585	0.17884	O	-2.51400	2.78967	-0.78325
H	3.38137	4.38087	-0.06650	H	-4.43016	2.10261	-0.33094
Pd	0.42519	-0.10093	-0.05680	C	-3.31977	0.09228	1.07766
C	-0.09417	-2.12443	0.03391	C	-4.80436	-0.31223	1.25912
C	-0.91529	-2.36854	-1.20686	H	-5.44097	0.53668	0.93013
C	-0.18736	-2.65829	-2.51661	H	1.48248	-1.27223	-2.41539
C	1.31980	-2.36938	-2.45163	H	1.82241	-2.74002	-3.36211
C	1.92581	-3.02656	-1.20443	H	3.02315	-2.92943	-1.16253
C	1.29602	-2.55496	0.10197	H	1.72632	-4.11987	-1.24573
H	-0.68704	-2.23645	0.95714	H	-0.36122	-3.73112	-2.73833
O	-2.14807	-2.38452	-1.13508	H	-0.69081	-2.09975	-3.32571
C	1.72334	-3.34610	1.32818	H	-2.67842	-0.74788	1.40472
H	1.28310	-2.95630	2.25877	H	-3.08776	0.95099	1.74016
H	1.34923	-4.38134	1.19555	C	-5.19208	-1.55179	0.43057
H	2.81902	-3.39078	1.43374	H	-6.23871	-1.83797	0.63517
C	2.32456	-0.73439	0.54060	H	-5.10475	-1.38298	-0.65719
C	2.47331	-0.52493	1.93693	H	-4.54756	-2.41346	0.68136
C	3.45610	-0.56425	-0.29488	C	-5.08862	-0.54320	2.75673
C	3.70764	-0.12905	2.47490	H	-6.15370	-0.78256	2.92145
H	1.61876	-0.66925	2.60856	H	-4.49253	-1.39074	3.14444
C	4.69828	-0.19664	0.25067	H	-4.84493	0.34837	3.36258

3-TS-B

E(Solv): -1359.105855

Correction to H: 0.531148

Correction to G: 0.440545

C	-1.22754	2.20736	-0.42451
C	-3.27828	2.00387	-1.28850
C	-2.81046	0.63635	-0.73459
N	-1.35975	0.90876	-0.46903
H	-4.26413	2.32854	-0.92792
C	0.02198	2.84943	-0.00110
C	0.17504	4.23684	0.11594
N	1.01960	1.96272	0.29052
C	1.40601	4.73600	0.56899
H	-0.65770	4.89670	-0.14181
C	2.20062	2.45306	0.71775
C	2.42938	3.83018	0.87760
H	1.56002	5.81405	0.67721
H	2.97519	1.71398	0.93890
H	3.40326	4.17453	1.23724
Pd	0.50233	-0.10116	-0.20960
C	0.09093	-2.01772	-0.94243
C	-1.17956	-2.49321	-0.29210
C	-1.09324	-3.12141	1.09670
C	0.27727	-2.92623	1.76171
C	1.39162	-3.33424	0.78863
C	1.38019	-2.54815	-0.51885
H	-0.04136	-1.85339	-2.02570
O	-2.24481	-2.42175	-0.91257
C	2.29307	-3.11424	-1.59563
H	2.29355	-2.50838	-2.51437
H	1.89773	-4.11503	-1.86270
H	3.32790	-3.24030	-1.23924
C	2.47272	-0.77364	-0.08175
C	3.23938	-0.33473	-1.19366
C	3.10186	-0.85018	1.18642
C	4.58527	0.03049	-1.03834
H	2.78167	-0.27562	-2.18797
C	4.45609	-0.50462	1.33487
H	2.53742	-1.17460	2.06691
C	5.20021	-0.06770	0.22375
H	5.15899	0.37483	-1.90576
H	4.92959	-0.57944	2.32018
H	6.25859	0.18914	0.33960
O	-2.28499	2.96402	-0.75399
H	-3.23186	2.07833	-2.38855
H	-2.89283	-0.17111	-1.47794
C	-3.51323	0.23260	0.58146
C	-5.03282	-0.05004	0.46417
H	-5.53740	0.88152	0.13028
H	1.23236	-4.39423	0.49231
H	2.39249	-3.30558	1.24966

H	0.39716	-1.86204	2.05174
H	0.34293	-3.52167	2.68910
H	-1.30585	-4.20193	0.96546
H	-1.92070	-2.72716	1.71337
H	-3.01008	-0.67083	0.97056
H	-3.34843	1.03769	1.32621
C	-5.36039	-1.16384	-0.54863
H	-6.44208	-1.38577	-0.53931
H	-5.09338	-0.88558	-1.58431
H	-4.81316	-2.09226	-0.30814
C	-5.59260	-0.39188	1.85949
H	-6.68662	-0.53380	1.81782
H	-5.14934	-1.32983	2.24374
H	-5.38282	0.40805	2.59279

3-TS-C

E(Solv): -1359.104270

Correction to H: 0.531267

Correction to G: 0.440659

C	-0.37101	2.47711	-0.49646
C	-2.56261	2.75580	-0.85383
C	-2.29802	1.32501	-0.30907
N	-0.80754	1.25609	-0.36275
H	-2.80373	2.78256	-1.92988
H	-2.71445	0.55317	-0.97665
C	1.05827	2.79625	-0.42572
C	1.56162	4.08994	-0.60488
N	1.85654	1.71273	-0.16856
C	2.94895	4.28709	-0.52068
H	0.87081	4.91290	-0.80726
C	3.19016	1.91116	-0.09671
C	3.76895	3.18192	-0.26495
H	3.37558	5.28601	-0.65413
H	3.79834	1.02697	0.13167
H	4.85525	3.28414	-0.18806
Pd	0.77251	-0.17317	-0.20823
C	2.32844	-1.57464	-0.03709
C	3.01713	-1.24069	1.25844
C	2.42167	-1.75663	2.56496
C	1.02109	-2.36406	2.39842
C	1.01489	-3.34408	1.21825
C	1.41732	-2.70716	-0.10621
H	2.97775	-1.41288	-0.91396
O	4.07879	-0.60451	1.24652
C	1.60923	-3.69337	-1.24594
H	1.85349	-3.19916	-2.19837
H	2.47242	-4.33559	-0.97739
H	0.73106	-4.34362	-1.38565
C	-0.40122	-1.78870	-0.80446
C	-0.47100	-1.78919	-2.22255
C	-1.52257	-2.23486	-0.06812
C	-1.63974	-2.20023	-2.88099

H	0.39256	-1.46995	-2.81821	H	-4.13027	1.98564	3.39727
C	-2.68050	-2.67388	-0.73191	H	-2.29375	1.88276	1.77811
H	-1.50149	-2.24404	1.02662				
C	-2.74293	-2.65579	-2.13629	**3-TS-D**			
H	-1.68009	-2.18673	-3.97574	E(Solv):	-1359.104018		
H	-3.53612	-3.03120	-0.14861	Correction to H:	0.531063		
H	-3.64418	-3.00722	-2.64977	Correction to G:	0.439144		
O	-1.27102	3.45550	-0.68634	C	0.34588	2.45725	0.49021
H	-3.31146	3.32655	-0.28628	C	2.33389	2.66982	1.49771
C	-2.77867	1.11313	1.14441	C	2.22011	1.25996	0.85088
C	-4.31226	1.16807	1.35989	N	0.78898	1.23286	0.42071
H	-4.68810	2.13357	0.96004	H	3.22094	3.23988	1.18594
H	0.71194	-2.87801	3.32540	C	-0.98377	2.83027	-0.00136
H	0.28608	-1.55211	2.21812	C	-1.41924	4.15801	-0.08376
H	0.05800	-3.88155	1.11411	N	-1.74225	1.76796	-0.41369
H	1.77795	-4.13160	1.40546	C	-2.67929	4.41596	-0.64587
H	2.44047	-0.93359	3.30151	H	-0.77095	4.96066	0.27784
H	3.12832	-2.52010	2.94896	C	-2.95084	2.02694	-0.95765
H	-2.39622	0.13414	1.49161	C	-3.44707	3.33534	-1.09542
C	-5.06002	0.03220	0.63680	H	-3.04856	5.44267	-0.73049
H	-6.14781	0.11509	0.80614	H	-3.55018	1.15641	-1.24419
H	-4.89665	0.03855	-0.45599	H	-4.43347	3.48406	-1.54388
H	-4.73833	-0.95404	1.02073	Pd	-0.74442	-0.14866	-0.19759
C	-4.61964	1.14704	2.87023	C	-2.29827	-1.49814	-0.63367
H	-5.70602	1.22138	3.05183	C	-3.45925	-1.07089	0.22327
H	-4.26714	0.20524	3.33148	C	-3.47645	-1.47530	1.69487

C	-2.15998	-2.11245	2.16436	H	-1.37598	-1.32992	2.23931
C	-1.72317	-3.19159	1.16649	H	-2.28006	-2.54670	3.17232
C	-1.51382	-2.66580	-0.24990	H	-2.53688	-3.94481	1.08016
H	-2.50984	-1.38490	-1.71051	H	-0.83706	-3.75358	1.50429
O	-4.39921	-0.44715	-0.28417	H	-3.75434	-0.58887	2.29308
C	-1.31644	-3.75674	-1.29040	H	-4.31437	-2.19167	1.81330
H	-1.13848	-3.35689	-2.29985	H	2.91157	0.06570	-0.81017
H	-2.25717	-4.34247	-1.32893	H	2.89905	1.81307	-1.12611
H	-0.49874	-4.44365	-1.01917	C	5.12129	0.08314	0.98973
C	0.44934	-1.85495	-0.24149	H	6.21232	0.14478	1.14765
C	1.04458	-2.01985	-1.52052	H	4.64221	0.23291	1.97480
C	1.17333	-2.27262	0.90234	H	4.88783	-0.94395	0.65372
C	2.31989	-2.59000	-1.65002	C	5.46105	0.95423	-1.36865
H	0.50161	-1.71483	-2.42285	H	6.54533	1.05889	-1.18909
C	2.44197	-2.85861	0.76879	H	5.28899	-0.04485	-1.81101
H	0.74593	-2.14874	1.90339	H	5.16826	1.71075	-2.11878
C	3.01223	-3.02839	-0.50637				
H	2.76284	-2.71274	-2.64443	**Complex 12 for TS4**			
H	2.98297	-3.19095	1.66169	E(Solv):	-1432.935662		
H	3.99092	-3.50933	-0.60892	Correction to H:	0.500123		
O	1.15395	3.40211	0.99729	Correction to G:	0.403879		
H	2.26140	2.66075	2.59821	C	2.54051	1.40232	-0.84895
H	2.37839	0.46437	1.59727	C	2.06902	3.53634	-1.36298
C	3.15007	1.04861	-0.36334	C	0.75141	2.77247	-0.98343
C	4.66801	1.11871	-0.05699	N	1.25412	1.41071	-0.65645
H	4.89932	2.12923	0.34097	H	2.32156	4.33313	-0.64588

C	3.33962	0.20086	-0.57959	H	-6.18016	0.56476	0.95358
C	4.72979	0.15514	-0.73465	H	-6.79579	0.59500	-0.73276
N	2.60640	-0.87206	-0.13355	H	-6.85840	-0.91122	0.19059
C	5.40744	-1.03054	-0.41332	C	0.14349	-2.39227	0.64901
H	5.25590	1.04281	-1.09606	C	-0.33113	-2.58215	1.96278
C	3.27083	-2.00813	0.18141	C	0.30467	-3.50876	-0.19970
C	4.66383	-2.12198	0.05332	C	-0.62154	-3.87959	2.42757
H	6.49427	-1.09537	-0.52215	H	-0.47529	-1.72484	2.63099
H	2.65216	-2.83613	0.53487	C	0.00135	-4.80283	0.26924
H	5.14612	-3.06586	0.32322	H	0.66482	-3.38094	-1.22840
Pd	0.56543	-0.53680	0.03002	C	-0.45754	-4.98981	1.58313
C	-3.73849	0.01743	0.09522	H	-0.97833	-4.01698	3.45497
C	-2.43243	-0.41713	-0.35588	H	0.12555	-5.66266	-0.39965
C	-2.32597	-1.31935	-1.56289	H	-0.68769	-5.99695	1.94706
C	-3.52294	-1.15418	-2.51576	O	3.13998	2.52397	-1.28287
C	-4.85504	-1.26317	-1.75338	H	0.08774	2.68255	-1.86329
C	-4.89383	-0.38860	-0.52048	H	2.07403	3.93421	-2.38865
H	-1.35684	-1.12938	-2.06012	C	-0.02704	3.41466	0.15390
H	-3.76458	0.64859	0.99039	C	-1.25235	4.05452	-0.11065
H	-3.46771	-0.16289	-3.00452	C	0.48563	3.42268	1.46723
H	-3.47508	-1.91120	-3.31714	C	-1.95492	4.69951	0.91994
H	-5.70739	-1.01379	-2.41243	H	-1.65560	4.05656	-1.13116
H	-5.03006	-2.31295	-1.43128	C	-0.22040	4.05919	2.49852
H	-2.26937	-2.35937	-1.17793	H	1.43589	2.92215	1.68963
O	-1.41781	-0.04403	0.31221	C	-1.44072	4.70124	2.22628
C	-6.24322	-0.00753	0.01449	H	-2.90310	5.20205	0.70051

H	0.18384	4.05592	3.51647
H	-1.98757	5.20353	3.03132

4-TS-A

E(Solv): -1432.905658

Correction to H: 0.498780

Correction to G: 0.409749

C	-1.47965	1.98323	-0.90592
C	-3.57406	1.41887	-1.47449
C	-2.83187	0.16642	-0.92115
N	-1.43087	0.68384	-0.80417
H	-3.73204	1.38278	-2.56476
H	-2.83557	-0.66128	-1.64695
C	-0.30320	2.81472	-0.62667
C	-0.29167	4.20974	-0.74993
N	0.77892	2.09594	-0.19843
C	0.88241	4.90001	-0.41034
H	-1.18735	4.72930	-1.10114
C	1.90012	2.76923	0.12784
C	1.99067	4.16873	0.03741
H	0.92673	5.99033	-0.49321
H	2.74149	2.15843	0.46732
H	2.92341	4.66634	0.31816
Pd	0.44489	-0.06863	-0.22245
C	0.10680	-2.12092	-0.37917
C	-0.38884	-2.32844	-1.78925
C	0.63401	-2.46159	-2.91399
C	2.06065	-2.08033	-2.49452
C	2.42405	-2.77812	-1.17700
C	1.48639	-2.43393	-0.02399
H	-0.66443	-2.34502	0.37596
O	-1.59877	-2.45050	-2.01240
C	1.70326	-3.26510	1.23120
H	1.04385	-2.96197	2.05883
H	1.44905	-4.31346	0.97563
H	2.75089	-3.24112	1.57101
C	2.25386	-0.57827	0.69780
C	2.10218	-0.44054	2.10277
C	3.50583	-0.25848	0.11726
C	3.15958	0.03259	2.89511
H	1.15009	-0.69878	2.58122
C	4.57212	0.18693	0.91789
H	3.65784	-0.34891	-0.96332
C	4.40109	0.33440	2.30600
H	3.01975	0.14652	3.97567
H	5.53743	0.41836	0.45374
H	5.23556	0.67426	2.92860
O	-2.65507	2.55153	-1.21501
H	-4.51805	1.64304	-0.95818
H	2.12557	-0.97990	-2.37037
H	2.78019	-2.35747	-3.28486
H	3.47407	-2.61410	-0.88391

H	2.32099	-3.87655	-1.31762
H	0.60122	-3.52224	-3.23695
H	0.27671	-1.87441	-3.77862
C	-3.33094	-0.34073	0.42640
C	-3.61177	-1.71087	0.59628
C	-3.52420	0.54354	1.50914
C	-4.08607	-2.18827	1.82950
H	-3.44808	-2.39790	-0.24110
C	-3.99483	0.06470	2.74067
H	-3.31786	1.61525	1.39286
C	-4.27716	-1.30308	2.90269
H	-4.31352	-3.25327	1.94812
H	-4.14913	0.76043	3.57250
H	-4.65194	-1.67493	3.86233

4-TS-B

E(Solv): -1432.903697

Correction to H: 0.498444

Correction to G: 0.409773

C	-1.07637	2.21197	-0.77149
C	-3.06503	2.00208	-1.77389
C	-2.61402	0.62171	-1.21238
N	-1.19673	0.91297	-0.82944
H	-4.07081	2.30747	-1.45498
C	0.12439	2.85152	-0.22032
C	0.28578	4.23946	-0.12207
N	1.06228	1.95944	0.21979
C	1.45968	4.73354	0.46780
H	-0.49594	4.90394	-0.50008
C	2.18855	2.44469	0.77966
C	2.41966	3.82276	0.92892
H	1.61875	5.81200	0.56386
H	2.91547	1.70014	1.11637
H	3.34603	4.16454	1.39945
Pd	0.60652	-0.10326	-0.34529
C	0.32102	-1.98349	-1.21094
C	-1.06981	-2.44589	-0.87019
C	-1.31109	-3.04663	0.51054
C	-0.10621	-2.88562	1.45108
C	1.17641	-3.34316	0.74268
C	1.47253	-2.56598	-0.53542
H	0.43400	-1.78751	-2.29120
O	-1.95703	-2.37399	-1.72695
C	2.56788	-3.17099	-1.39977
H	2.78674	-2.56665	-2.29282
H	2.19786	-4.15525	-1.75121
H	3.49828	-3.33853	-0.83381
C	2.51340	-0.81877	0.09957
C	3.47708	-0.39452	-0.85323
C	2.90086	-0.91321	1.45997
C	4.78008	-0.05928	-0.45408
H	3.20884	-0.32419	-1.91396

C	4.21179	-0.59465	1.85396
H	2.17953	-1.23086	2.22062
C	5.15339	-0.17106	0.89822
H	5.50911	0.27353	-1.20111
H	4.49735	-0.68088	2.90830
H	6.17809	0.06408	1.20529
O	-2.10661	2.96479	-1.18709
H	-2.96419	2.08077	-2.86965
H	-2.62326	-0.15722	-1.99092
H	1.04650	-4.39911	0.41900
H	2.05484	-3.34838	1.40929
H	-0.01228	-1.81971	1.74922
H	-0.26117	-3.46627	2.37719
H	-1.53723	-4.12101	0.35474
H	-2.23198	-2.59854	0.92436
C	-3.43833	0.15524	-0.01458
C	-4.30744	-0.94535	-0.15604
C	-3.40870	0.85367	1.21096
C	-5.13702	-1.33532	0.90820
H	-4.31680	-1.50966	-1.09416
C	-4.23385	0.45924	2.27524
H	-2.74270	1.71481	1.34293
C	-5.10176	-0.63544	2.12541
H	-5.81081	-2.18993	0.78405
H	-4.20233	1.01107	3.22093
H	-5.74863	-0.94087	2.95471

4-TS-C

E(Solv): -1432.903112

Correction to H: 0.498737

Correction to G: 0.409281

C	0.27718	2.47491	-0.73564
C	-1.76133	3.21673	-1.29819
C	-1.84889	1.72370	-0.83075
N	-0.41382	1.37156	-0.67092
H	-1.91364	3.34289	-2.38274
H	-2.28090	1.09213	-1.62566
C	1.72511	2.48183	-0.50237
C	2.51620	3.62829	-0.63961
N	2.23389	1.26027	-0.14519
C	3.89698	3.52056	-0.40989
H	2.04874	4.57458	-0.92524
C	3.56367	1.16620	0.06947
C	4.42265	2.27310	-0.05344
H	4.54496	4.39681	-0.50977
H	3.93212	0.18072	0.38042
H	5.49123	2.13921	0.13789
Pd	0.77826	-0.35175	-0.28335
C	1.93298	-2.05341	0.15661
C	2.50864	-1.76910	1.51675
C	1.65008	-2.03885	2.74889
C	0.17627	-2.31392	2.41567

C	0.08140	-3.36042	1.29810	H	2.09968	-2.91782	3.25432
C	0.79625	-2.95137	0.01695	C	-2.65111	1.53279	0.45216
H	2.70580	-2.11232	-0.62801	C	-4.01119	1.17455	0.36011
O	3.67790	-1.37624	1.62261	C	-2.09085	1.77936	1.72128
C	0.89196	-4.04856	-1.02960	C	-4.80003	1.06841	1.51589
H	1.37057	-3.70736	-1.96011	H	-4.45598	0.98075	-0.62366
H	1.53166	-4.84839	-0.60433	C	-2.87846	1.66429	2.87865
H	-0.09120	-4.48698	-1.26357	H	-1.03481	2.05798	1.81211
C	-0.64060	-1.69996	-0.98960	C	-4.23387	1.31049	2.77874
C	-0.51151	-1.80634	-2.39925	H	-5.85702	0.79431	1.43015
C	-1.92654	-1.80050	-0.41071	H	-2.43236	1.85837	3.86013
C	-1.64380	-1.98874	-3.20737	H	-4.84782	1.22571	3.68156
H	0.47762	-1.74967	-2.86895				
C	-3.05439	-2.00930	-1.22233	**4-TS-D**			
H	-2.06239	-1.70040	0.67058	E(Solv):	-1432.901894		
C	-2.91651	-2.10425	-2.61803	Correction to H:	0.498516		
H	-1.52978	-2.06263	-4.29449	Correction to G:	0.408927		
H	-4.04315	-2.09344	-0.75849	C	0.27155	2.36595	0.82529
H	-3.79701	-2.27780	-3.24601	C	2.13680	2.42772	2.06115
O	-0.36971	3.61743	-1.01239	C	2.02836	1.04786	1.33047
H	-2.41887	3.89532	-0.73690	N	0.66723	1.12634	0.73446
H	-0.36181	-2.66412	3.31394	H	3.08159	2.95647	1.87321
H	-0.31388	-1.37176	2.09286	C	-0.97329	2.82146	0.19842
H	-0.95759	-3.65788	1.08061	C	-1.35242	4.16804	0.15024
H	0.59227	-4.28940	1.63465	N	-1.70304	1.81683	-0.37979
H	1.77569	-1.19368	3.44893	C	-2.51920	4.51032	-0.55153

H	-0.73294	4.92036	0.64595	C	2.88588	-3.09981	0.10932
C	-2.81975	2.15785	-1.05765	H	3.03023	-2.70847	-2.02398
C	-3.25274	3.49125	-1.16985	H	2.46517	-3.33765	2.22973
H	-2.84238	5.55405	-0.61354	H	3.86467	-3.58742	0.16733
H	-3.40037	1.33140	-1.48226	O	1.05286	3.24062	1.47776
H	-4.16522	3.70686	-1.73306	H	1.93977	2.36407	3.14444
Pd	-0.81018	-0.15603	-0.14160	H	2.05086	0.21953	2.05866
C	-2.31271	-1.43564	-0.87597	H	-1.87639	-1.38907	2.11631
C	-3.58380	-0.99065	-0.20610	H	-2.95747	-2.60469	2.83864
C	-3.85879	-1.44423	1.22516	H	-2.89546	-3.92974	0.68750
C	-2.65828	-2.14168	1.88202	H	-1.28415	-3.79857	1.38946
C	-2.09004	-3.20231	0.93079	H	-4.20690	-0.56927	1.80299
C	-1.64014	-2.64062	-0.41260	H	-4.72480	-2.13477	1.17420
H	-2.33505	-1.27697	-1.96754	C	3.12501	0.83300	0.29333
O	-4.40501	-0.31085	-0.83418	C	4.30301	0.16435	0.68115
C	-1.29114	-3.69707	-1.44705	C	3.03267	1.36384	-1.00789
H	-0.93558	-3.26260	-2.39314	C	5.37533	0.03406	-0.21460
H	-2.22411	-4.25376	-1.66991	H	4.38401	-0.25340	1.69218
H	-0.54630	-4.41706	-1.07191	C	4.10175	1.22426	-1.90735
C	0.33783	-1.88531	-0.04701	H	2.12065	1.88047	-1.32773
C	1.14509	-2.02580	-1.20568	C	5.27577	0.56242	-1.51232
C	0.83567	-2.35561	1.19267	H	6.28838	-0.48197	0.10140
C	2.41403	-2.61654	-1.12346	H	4.01856	1.63913	-2.91776
H	0.77995	-1.67688	-2.17873	H	6.11165	0.46082	-2.21260
C	2.09845	-2.96410	1.26692				
H	0.23841	-2.25190	2.10498	**Complex 12 for TS5**			

E(Solv): -1696.161800

Correction to H: 0.539743

Correction to G: 0.433322

C	-1.57063	1.68654	0.54091	H	4.24701	0.54717	2.93835
C	-1.08925	3.77390	1.17914	H	4.16609	-1.12773	3.52318
C	0.09675	3.18476	0.35720	H	6.48594	-0.44661	2.65189
N	-0.31796	1.76160	0.19615	H	5.82893	-1.86939	1.84423
H	-1.48364	4.72643	0.79881	H	3.08324	-1.87998	1.40346
C	-2.34499	0.45328	0.35427	O	2.42842	0.18145	-0.49662
C	-3.72060	0.37589	0.58909	C	7.22203	0.13018	0.13748
N	-1.61082	-0.60848	-0.11452	H	7.24521	0.53747	-0.88569
C	-4.38528	-0.82786	0.30608	H	7.74688	0.83421	0.81247
H	-4.25244	1.24593	0.98248	H	7.81079	-0.80728	0.15999
C	-2.26372	-1.76157	-0.38930	C	0.87198	-2.16696	-0.65872
C	-3.64519	-1.90577	-0.19659	C	1.42282	-2.50353	-1.91146
H	-1.64569	-2.58277	-0.75801	C	0.65040	-3.17794	0.30082
H	-4.12599	-2.85894	-0.43086	C	1.73038	-3.84600	-2.20666
Pd	0.41931	-0.25528	-0.28238	H	1.61220	-1.72864	-2.66351
C	4.73089	0.21559	-0.12485	C	0.97147	-4.51715	0.00110
C	3.38275	-0.10465	0.29407	H	0.22614	-2.93417	1.28293
C	3.15953	-0.79337	1.61957	C	1.50749	-4.85235	-1.25260
C	4.29626	-0.51082	2.61773	H	2.14644	-4.09998	-3.18843
C	5.67128	-0.77716	1.98098	H	0.79928	-5.29519	0.75404
C	5.82663	-0.11726	0.62957	H	1.75121	-5.89448	-1.48538
H	2.16918	-0.49222	2.00869	O	-2.17136	2.77805	1.04234
H	4.84331	0.68711	-1.10753	H	1.03123	3.21022	0.94605
				H	-0.87452	3.86406	2.25691
				C	0.36989	3.89850	-1.01318
				C	1.51534	3.17153	-1.74983

H	2.43478	3.14182	-1.13712
H	1.24364	2.13318	-2.00461
H	1.75442	3.70188	-2.68881
C	0.81421	5.34945	-0.70953
H	1.06210	5.86860	-1.65193
H	0.02644	5.94415	-0.21202
H	1.71551	5.37268	-0.06927
C	-0.89053	3.90569	-1.90584
H	-1.21413	2.88002	-2.15931
H	-1.74168	4.43449	-1.43911
H	-0.67203	4.42393	-2.85575
C	-5.89178	-0.92675	0.49256
F	-6.28053	-2.21369	0.65935
F	-6.52962	-0.42852	-0.59674
F	-6.28894	-0.21088	1.57455

5-TS-A

E(Solv): -1696.129336

Correction to H: 0.538360

Correction to G: 0.438455

C	-1.00779	1.82445	0.40785
C	-0.33531	3.90136	0.87965
C	0.80624	3.14001	0.15434
N	0.27054	1.74307	0.15532
H	-0.16185	4.03069	1.96120
H	1.73920	3.15243	0.74156
C	-1.89748	0.66263	0.28457
C	-3.28327	0.73670	0.46157
N	-1.25039	-0.49017	-0.06178
C	-4.04350	-0.42400	0.24623
H	-3.74810	1.67995	0.75923
C	-1.99184	-1.59722	-0.26661
C	-3.38904	-1.60499	-0.12925
H	-1.44172	-2.50136	-0.54019
H	-3.94918	-2.52697	-0.30516
Pd	0.92089	-0.28112	-0.04864
C	3.00406	-0.11432	0.12429
C	3.20465	0.74088	1.34999
C	3.15165	0.07306	2.72185
C	2.63159	-1.37170	2.67782
C	3.36230	-2.15763	1.58123
C	3.20429	-1.55483	0.19057
H	3.33917	0.38416	-0.79856
O	3.46087	1.94370	1.22813
C	4.07700	-2.19406	-0.87694
H	3.91063	-1.76293	-1.87580
H	5.13148	-1.98950	-0.60182
H	3.94375	-3.28670	-0.92332
C	1.30655	-2.28241	-0.48812
C	1.27332	-2.45716	-1.89704
C	0.84348	-3.33569	0.33837
C	0.76098	-3.63643	-2.46027

H	1.64794	-1.66742	-2.55901	H	4.18739	0.09436	3.11788
C	0.36255	-4.52847	-0.22836	H	2.55992	0.71474	3.39893
H	0.84918	-3.23073	1.42850	C	-5.56008	-0.37530	0.36566
C	0.31832	-4.67993	-1.62633	F	-6.10541	0.01833	-0.81284
H	0.72784	-3.74909	-3.54940	F	-5.93987	0.50835	1.32137
H	0.02002	-5.33892	0.42473	F	-6.06379	-1.59360	0.67893
H	-0.05111	-5.61288	-2.06515				
O	-1.51641	3.01652	0.74412	**5-TS-B**			
H	-0.60795	4.86425	0.42715	E(Solv):	-1696.126030		
C	1.12927	3.67344	-1.28866	Correction to H:	0.538530		
C	2.19980	2.77659	-1.94779	Correction to G:	0.439968		
H	1.81382	1.75623	-2.12608	C	0.95270	1.78160	-0.64279
H	2.49545	3.19890	-2.92471	C	0.19937	3.67553	-1.54809
H	3.09962	2.70588	-1.31204	C	-0.90004	3.05749	-0.65064
C	-0.12864	3.71408	-2.18366	N	-0.32984	1.69267	-0.40641
H	-0.55949	2.70643	-2.32976	H	0.42341	4.73166	-1.34882
H	-0.91849	4.37479	-1.78248	C	1.88508	0.71047	-0.26570
H	0.13726	4.10136	-3.18295	C	3.27605	0.83245	-0.35478
C	1.71481	5.09804	-1.13125	N	1.26525	-0.40152	0.22968
H	2.62100	5.09431	-0.49907	C	4.06541	-0.22781	0.11893
H	1.99764	5.49567	-2.12172	H	3.72267	1.73393	-0.78154
H	0.99304	5.81116	-0.69292	C	2.03329	-1.41718	0.67128
H	1.54104	-1.36574	2.47118	C	3.43580	-1.36412	0.64595
H	2.77122	-1.86073	3.65779	H	1.50047	-2.29283	1.05266
H	3.09704	-3.22762	1.57325	H	4.02107	-2.20695	1.02252
H	4.45469	-2.12574	1.78811	Pd	-0.88205	-0.36917	-0.16338

C	-2.80555	-0.43266	-0.98106	C	-1.14634	3.85631	0.68498
C	-3.66062	0.62382	-0.33558	C	-1.77795	5.21614	0.29816
C	-4.40961	0.26382	0.94247	H	-1.09560	5.85391	-0.29265
C	-3.90034	-1.03189	1.58976	H	-2.03329	5.78022	1.21236
C	-3.86508	-2.15875	0.54858	H	-2.70795	5.07663	-0.28203
C	-2.99680	-1.84342	-0.66575	C	-2.14472	3.09495	1.58239
H	-2.59812	-0.19634	-2.03974	H	-1.76907	2.08830	1.84279
O	-3.79004	1.72374	-0.88363	H	-3.11915	2.99030	1.07680
C	-3.19368	-2.79098	-1.83914	H	-2.30047	3.65126	2.52384
H	-2.53189	-2.56051	-2.68802	C	0.16406	4.08898	1.47020
H	-4.23533	-2.65372	-2.19273	H	0.91742	4.65395	0.89260
H	-3.06779	-3.84667	-1.55077	H	0.61980	3.13727	1.80005
C	-1.04704	-2.44707	-0.06179	H	-0.05118	4.67585	2.38038
C	-0.35662	-3.10539	-1.11349	H	-4.89161	-2.29581	0.14338
C	-1.03566	-3.03766	1.22774	H	-3.58736	-3.13324	0.98274
C	0.32763	-4.30824	-0.88132	H	-2.88564	-0.85859	2.00202
H	-0.35058	-2.67511	-2.12124	H	-4.54612	-1.31846	2.43809
C	-0.35815	-4.24811	1.45509	H	-5.47719	0.15651	0.66018
H	-1.55348	-2.55624	2.06370	H	-4.36579	1.12450	1.63197
C	0.31833	-4.88838	0.40074	C	5.58318	-0.11436	0.10878
H	0.85673	-4.80008	-1.70495	F	6.01179	0.47071	1.25555
H	-0.36597	-4.69318	2.45625	F	6.16162	-1.33664	0.01650
H	0.83129	-5.84003	0.57608	F	6.00467	0.64321	-0.93377
O	1.42006	2.90628	-1.20000				
H	0.02829	3.52206	-2.62738	**5-TS-C**			
H	-1.86030	2.94623	-1.18070	E(Solv):	-1696.125752		

Correction to H:	0.538393		
Correction to G:	0.438874		
C	1.10905	1.63476	-0.27514
C	0.31072	3.66791	-0.73785
C	-0.77241	2.83761	0.00276
N	-0.15945	1.47480	-0.01773
H	0.12119	3.77434	-1.81937
H	-1.71560	2.80592	-0.56910
C	2.06015	0.51937	-0.19989
C	3.43444	0.68150	-0.39871
N	1.48411	-0.68719	0.09790
C	4.26376	-0.44470	-0.27279
H	3.83817	1.66528	-0.65068
C	2.28989	-1.76533	0.20400
C	3.68236	-1.68124	0.03288
H	1.79402	-2.71445	0.44752
H	4.29295	-2.58243	0.13341
Pd	-0.68789	-0.61581	-0.06648
C	-1.15652	-2.66154	-0.14325
C	-0.72455	-3.18855	1.20084
C	-1.68162	-3.07075	2.38215
C	-2.88115	-2.15366	2.10679
C	-3.52268	-2.51854	0.76212
C	-2.56525	-2.42923	-0.41815
H	-0.55635	-3.07123	-0.97296
O	0.36523	-3.76413	1.31692
C	-3.12360	-2.95254	-1.72898
H	-2.42477	-2.82481	-2.56963
H	-3.28862	-4.04166	-1.60013
H	-4.09050	-2.49022	-1.98325
C	-2.57195	-0.31176	-0.90792
C	-2.39225	-0.10715	-2.30147
C	-3.62772	0.35915	-0.25205
C	-3.22351	0.77646	-3.00654
H	-1.60049	-0.63988	-2.84169
C	-4.47444	1.22420	-0.96671
H	-3.79543	0.21834	0.81972
C	-4.27255	1.43747	-2.34133
H	-3.06689	0.92983	-4.07999
H	-5.29497	1.73006	-0.44553
H	-4.94019	2.10455	-2.89697
O	1.54356	2.86154	-0.60015
H	0.52231	4.65116	-0.29687
C	-1.08134	3.34601	1.45878
C	-2.06618	2.38283	2.15397
H	-1.64956	1.36202	2.22578
H	-2.28035	2.73646	3.17817
H	-3.02420	2.33089	1.60812
C	0.20342	3.45397	2.31053
H	0.68989	2.47066	2.44343
H	0.94389	4.15359	1.88323
H	-0.05023	3.82942	3.31725

C	-1.75252	4.73558	1.33815
H	-2.67353	4.68934	0.72833
H	-2.03363	5.10279	2.34067
H	-1.08570	5.49576	0.89253
H	-3.62342	-2.23821	2.91966
H	-2.54256	-1.09765	2.08919
H	-4.44161	-1.94477	0.55795
H	-3.84040	-3.58431	0.79624
H	-1.10137	-2.75647	3.26786
H	-2.02915	-4.10102	2.60144
C	5.77187	-0.30045	-0.41688
F	6.08009	0.67879	-1.30417
F	6.32226	0.02811	0.77916
F	6.33483	-1.45768	-0.83874

5-TS-D

E(Solv): -1696.124707

Correction to H: 0.538200

Correction to G: 0.438291

C	-1.04502	1.46326	0.75324
C	-0.22592	3.15652	1.95337
C	0.81771	2.70793	0.89758
N	0.21224	1.43104	0.40348
H	-0.44938	4.23170	1.95389
C	-2.01133	0.47626	0.25647
C	-3.39435	0.65275	0.35603
N	-1.43710	-0.59204	-0.37714
C	-4.23148	-0.28505	-0.27125
H	-3.79880	1.50887	0.90195
C	-2.25209	-1.48582	-0.97572
C	-3.65126	-1.35915	-0.95600
H	-1.77003	-2.35325	-1.43481
H	-4.26852	-2.11000	-1.45559
Pd	0.72798	-0.59155	-0.25278
C	1.17003	-2.61939	-0.60371
C	0.16403	-3.38522	0.21658
C	0.40515	-3.53505	1.71664
C	1.58010	-2.68863	2.22994
C	2.80007	-2.89284	1.32438
C	2.54791	-2.53323	-0.13587
H	1.03378	-2.78158	-1.68668
O	-0.80310	-3.91477	-0.34135
C	3.65219	-2.98184	-1.07857
H	3.46187	-2.70070	-2.12468
H	3.68412	-4.08953	-1.03554
H	4.63990	-2.60267	-0.77036
C	2.80006	-0.42039	-0.25681
C	3.31666	-0.11005	-1.54260
C	3.48448	0.06655	0.88588
C	4.48375	0.65521	-1.68032
H	2.81327	-0.48395	-2.44199
C	4.65625	0.82602	0.74562

H	3.10691	-0.15549	1.89041
C	5.16415	1.10991	-0.53630
H	4.87049	0.88408	-2.67926
H	5.18092	1.18696	1.63732
H	6.09251	1.68131	-0.64239
O	-1.46491	2.45792	1.55082
H	0.00813	2.82128	2.97838
H	1.79168	2.47786	1.36253
C	1.05207	3.75707	-0.24826
C	1.76019	4.98165	0.38027
H	1.14251	5.49032	1.14296
H	1.98202	5.72695	-0.40345
H	2.71909	4.69703	0.85147
C	1.97143	3.15006	-1.32518
H	1.50248	2.27879	-1.81338
H	2.93405	2.82503	-0.89488
H	2.18589	3.90230	-2.10524
C	-0.27465	4.19765	-0.90738
H	-0.96798	4.68417	-0.19817
H	-0.79883	3.34726	-1.38039
H	-0.06339	4.93062	-1.70551
H	1.29364	-1.61577	2.23416
H	1.82510	-2.96134	3.27135
H	3.06055	-3.97392	1.31734
H	3.70044	-2.37779	1.69796
H	-0.53986	-3.30880	2.24265
H	0.59822	-4.61158	1.89795
C	-5.74030	-0.08843	-0.24644
F	-6.39197	-1.25463	-0.46510
F	-6.13841	0.41282	0.94987
F	-6.10727	0.79183	-1.21255

Complex 12 for TS6

E(Solv): -1473.665086

Correction to H: 0.566472

Correction to G: 0.464947

C	1.96193	1.61657	-0.62164
C	1.49541	3.71564	-1.23415
C	0.32997	3.14518	-0.37164
N	0.72339	1.71440	-0.23261
H	1.91867	4.66101	-0.86697
C	2.71721	0.36550	-0.47470
C	4.07545	0.27207	-0.75470
N	1.97184	-0.68529	0.00939
C	4.74350	-0.95318	-0.51159
H	4.62444	1.13244	-1.14522
C	2.62061	-1.84805	0.24627
C	3.98830	-2.02609	0.00903
H	2.00528	-2.66448	0.63069
H	4.43680	-2.99646	0.23234
Pd	-0.04396	-0.28670	0.25291
C	-4.34578	0.29397	0.23230

C	-3.01415	-0.04516	-0.22718	H	-0.57949	-5.29772	-0.84759
C	-2.83993	-0.69661	-1.57916	H	-1.48372	-5.91138	1.40783
C	-3.98449	-0.33809	-2.54342	O	2.56329	2.70228	-1.13829
C	-5.35571	-0.58580	-1.89123	H	-0.62511	3.19224	-0.92525
C	-5.46495	0.02251	-0.51094	H	1.24228	3.81272	-2.30319
H	-1.84573	-0.41946	-1.97599	C	0.12224	3.86005	1.00942
H	-4.42437	0.73024	1.23448	C	-1.00609	3.15107	1.78881
H	-3.90661	0.73000	-2.82252	H	-1.94833	3.13704	1.21109
H	-3.89133	-0.92167	-3.47529	H	-0.74169	2.10803	2.03142
H	-6.17103	-0.20093	-2.53197	H	-1.20089	3.68384	2.73676
H	-5.54702	-1.67712	-1.79686	C	-0.30838	5.31917	0.72692
H	-2.80135	-1.79227	-1.40252	H	-0.51115	5.84046	1.67893
O	-2.03570	0.19254	0.54799	H	0.46940	5.90128	0.19970
C	-6.84335	0.28925	0.01866	H	-1.23330	5.35908	0.12200
H	-6.83474	0.65408	1.05802	C	1.41630	3.84224	1.85257
H	-7.36012	1.03577	-0.61564	H	1.73178	2.80964	2.08697
H	-7.45981	-0.62922	-0.02968	H	2.25711	4.35844	1.35408
C	-0.52712	-2.19162	0.61816	H	1.24399	4.35930	2.81273
C	-1.04992	-2.53838	1.88080	O	6.05674	-0.97832	-0.79842
C	-0.36014	-3.19341	-0.36237	C	6.78791	-2.20096	-0.56180
C	-1.38521	-3.87690	2.16271	H	7.82030	-1.98186	-0.86525
H	-1.19632	-1.77212	2.65115	H	6.76207	-2.47253	0.50848
C	-0.70867	-4.52866	-0.07677	H	6.38375	-3.02464	-1.17672
H	0.04423	-2.94296	-1.35114				
C	-1.21780	-4.87220	1.18590	**6-TS-A**			
H	-1.77985	-4.13702	3.15184	E(Solv):	-1473.633161		

Correction to H:	0.565260		
Correction to G:	0.470748		
C	0.81435	2.11747	-0.49257
C	-0.40459	3.93017	-0.96106
C	-1.27172	2.91590	-0.17001
N	-0.38653	1.71085	-0.17902
H	-0.65226	3.97677	-2.03510
H	-2.20063	2.66898	-0.71031
C	1.98142	1.23116	-0.39729
C	3.28166	1.66722	-0.62717
N	1.66492	-0.04556	-0.01099
C	4.34788	0.75420	-0.43195
H	3.48454	2.69369	-0.94249
C	2.68738	-0.90306	0.17880
C	4.03185	-0.55559	-0.00939
H	2.41337	-1.91419	0.49200
H	4.80349	-1.30619	0.17388
Pd	-0.48126	-0.40728	0.05256
C	-2.54086	-0.78290	-0.03494
C	-3.01761	-0.02264	-1.24362
C	-2.84606	-0.65790	-2.62170
C	-1.95713	-1.91029	-2.61062
C	-2.40144	-2.85601	-1.48706
C	-2.33957	-2.22463	-0.09986
H	-2.95544	-0.38513	0.90398
O	-3.58416	1.06774	-1.10532
C	-2.97205	-3.06600	0.99860
H	-2.87073	-2.60845	1.99443
H	-4.05595	-3.13340	0.77562
H	-2.56425	-4.08925	1.02416
C	-0.30752	-2.44123	0.48572
C	-0.16343	-2.61214	1.88857
C	0.38605	-3.32542	-0.37710
C	0.66926	-3.61575	2.40771
H	-0.70326	-1.95613	2.58169
C	1.19224	-4.35066	0.14564
H	0.30849	-3.21402	-1.46367
C	1.33602	-4.49747	1.53713
H	0.77966	-3.72312	3.49237
H	1.71070	-5.03347	-0.53687
H	1.95897	-5.30190	1.94263
O	0.97250	3.39431	-0.86693
H	-0.37977	4.94414	-0.53975
C	-1.65909	3.38351	1.27951
C	-2.42472	2.25544	2.00573
H	-1.77330	1.38240	2.19265
H	-2.78824	2.61798	2.98392
H	-3.29499	1.92480	1.41230
C	-0.41668	3.77699	2.10795
H	0.27019	2.92096	2.24126
H	0.15023	4.61087	1.65578
H	-0.72776	4.10651	3.11504

C	-2.60742	4.59871	1.13196
H	-3.50285	4.34087	0.53779
H	-2.94950	4.92850	2.12872
H	-2.11817	5.46809	0.65593
H	-0.90054	-1.61015	-2.45140
H	-2.00423	-2.42461	-3.58654
H	-1.86187	-3.81734	-1.50060
H	-3.47215	-3.11355	-1.64185
H	-3.86549	-0.91546	-2.97429
H	-2.47529	0.11585	-3.31756
O	5.58261	1.23072	-0.66691
C	6.70977	0.34774	-0.47947
H	7.59207	0.95060	-0.73246
H	6.77486	0.01210	0.57078
H	6.64389	-0.52187	-1.15738

6-TS-B

E(Solv): -1473.629400

Correction to H: 0.565004

Correction to G: 0.470855

C	0.66973	2.12677	-0.64065
C	-0.64436	3.67395	-1.56490
C	-1.49304	2.74949	-0.66003
N	-0.51987	1.63845	-0.40257
H	-0.77122	4.74896	-1.38097
C	1.89359	1.40339	-0.26964
C	3.16227	1.96651	-0.35398
N	1.65210	0.14426	0.21467
C	4.26927	1.21314	0.11045
H	3.30850	2.97112	-0.75835
C	2.71290	-0.56701	0.64460
C	4.02607	-0.07853	0.62722
H	2.49630	-1.57167	1.01939
H	4.83152	-0.70986	1.00812
Pd	-0.39344	-0.49236	-0.17056
C	-2.21843	-1.15809	-0.95274
C	-3.34547	-0.41606	-0.29271
C	-3.90451	-0.96554	1.01556
C	-3.00105	-2.03003	1.65477
C	-2.64674	-3.10464	0.61843
C	-1.94947	-2.55213	-0.62229
H	-2.11746	-0.88295	-2.01731
O	-3.83507	0.57469	-0.84713
C	-1.87568	-3.53395	-1.78250
H	-1.33711	-3.12596	-2.65150
H	-2.91739	-3.72958	-2.10714
H	-1.42321	-4.49454	-1.48871
C	0.10369	-2.51800	-0.08746
C	0.93754	-2.91958	-1.16457
C	0.33269	-3.08771	1.19069
C	1.96852	-3.85037	-0.96698
H	0.78328	-2.50002	-2.16525

C	1.35762	-4.02971	1.38381	H	-4.89633	-1.40036	0.77475
H	-0.28770	-2.79581	2.04419	H	-4.10354	-0.12007	1.69638
C	2.17285	-4.41706	0.30484	O	5.47016	1.81018	0.01534
H	2.60377	-4.14458	-1.80978	C	6.63462	1.09414	0.48018
H	1.51377	-4.46485	2.37724	H	7.47893	1.77419	0.30524
H	2.96024	-5.16397	0.45272	H	6.55267	0.86933	1.55844
O	0.75429	3.33927	-1.20577	H	6.77874	0.16303	-0.09633
H	-0.75377	3.45936	-2.64199				
H	-2.36866	2.33542	-1.18647	**6-TS-C**			
C	-1.98198	3.44724	0.66519	E(Solv):	-1473.629382		
C	-3.00714	4.53572	0.26295	Correction to H:	0.565078		
H	-2.55903	5.34636	-0.34036	Correction to G:	0.470151		
H	-3.42658	5.00575	1.17000	C	1.33384	1.75234	-0.37859
H	-3.84728	4.10450	-0.31104	C	0.36326	3.71401	-0.82112
C	-2.69461	2.42344	1.57338	C	-0.61939	2.81424	-0.02545
H	-2.02340	1.58762	1.84328	N	0.09134	1.50131	-0.06825
H	-3.58664	2.01420	1.07062	H	0.11836	3.78881	-1.89434
H	-3.01760	2.91400	2.50902	H	-1.58380	2.71063	-0.55138
C	-0.81354	4.08701	1.44828	C	2.36660	0.71074	-0.33132
H	-0.27350	4.85516	0.86618	C	3.71052	0.97810	-0.56574
H	-0.08342	3.32820	1.78456	N	1.88274	-0.53330	-0.00632
H	-1.20555	4.58333	2.35341	C	4.64515	-0.08142	-0.45261
H	-3.59097	-3.55787	0.24451	H	4.04595	1.98476	-0.82717
H	-2.06967	-3.93970	1.04855	C	2.78002	-1.53807	0.08622
H	-2.07847	-1.54633	2.03534	C	4.15548	-1.36121	-0.11708
H	-3.50357	-2.49048	2.52346	H	2.37230	-2.52337	0.34699

H	4.81532	-2.22475	-0.00907	H	0.51642	4.71761	-0.40188
Pd	-0.28249	-0.61971	-0.09589	C	-0.89322	3.31162	1.44138
C	-0.59163	-2.69446	-0.17264	C	-1.75789	2.27934	2.19479
C	-0.07055	-3.21629	1.13921	H	-1.25097	1.29984	2.25885
C	-0.97613	-3.17047	2.36573	H	-1.95309	2.63080	3.22362
C	-2.24721	-2.33534	2.15637	H	-2.73188	2.13619	1.69601
C	-2.91865	-2.72922	0.83445	C	0.42092	3.53110	2.22477
C	-2.02249	-2.54543	-0.38348	H	0.99368	2.59243	2.33385
H	-0.00138	-3.04797	-1.03441	H	1.07793	4.28624	1.75734
O	1.05366	-3.73186	1.19799	H	0.18958	3.89092	3.24267
C	-2.59993	-3.08936	-1.67896	C	-1.67990	4.64115	1.34868
H	-1.95208	-2.89518	-2.54733	H	-2.62556	4.51393	0.79033
H	-2.67615	-4.18976	-1.56455	H	-1.93506	4.99616	2.36263
H	-3.60908	-2.69689	-1.88117	H	-1.10216	5.44719	0.86115
C	-2.23004	-0.43615	-0.83559	H	-2.94593	-2.47941	2.99905
C	-2.14671	-0.18710	-2.23087	H	-1.98138	-1.25873	2.13659
C	-3.29742	0.13550	-0.10832	H	-3.88715	-2.22553	0.68071
C	-3.08383	0.64108	-2.86742	H	-3.15002	-3.81706	0.86231
H	-1.34541	-0.64077	-2.82635	H	-0.37651	-2.82130	3.22517
C	-4.24917	0.94485	-0.75317	H	-1.24253	-4.22293	2.59255
H	-3.39347	-0.03947	0.96732	O	5.93077	0.23845	-0.67970
C	-4.14353	1.20173	-2.13073	C	6.92652	-0.80255	-0.57037
H	-2.99926	0.82970	-3.94347	H	7.88267	-0.30998	-0.79173
H	-5.07569	1.37299	-0.17481	H	6.94727	-1.21887	0.45237
H	-4.89165	1.82472	-2.63249	H	6.73847	-1.60389	-1.30675
O	1.65813	3.00730	-0.72810				

6-TS-D

E(Solv): -1473.628237

Correction to H: 0.564949

Correction to G: 0.470326

C	-1.19520	1.65061	0.74799
C	-0.15743	3.25455	1.90135
C	0.79944	2.68140	0.82478
N	0.04383	1.47032	0.37642
H	-0.25770	4.34833	1.89769
C	-2.27704	0.77640	0.27903
C	-3.62031	1.10366	0.42433
N	-1.83267	-0.33884	-0.38602
C	-4.59228	0.26853	-0.18202
H	-3.92579	1.99574	0.97661
C	-2.76623	-1.11930	-0.97014
C	-4.14061	-0.85394	-0.90765
H	-2.40043	-2.02098	-1.46925
H	-4.82913	-1.53595	-1.41070
Pd	0.31255	-0.59487	-0.26536
C	0.50764	-2.65245	-0.65802
C	-0.60119	-3.32766	0.10394
C	-0.43514	-3.53165	1.60835
C	0.80200	-2.82464	2.18239
C	2.02670	-3.14262	1.31652
C	1.86889	-2.72534	-0.14220
H	0.39403	-2.77050	-1.74928
O	-1.59563	-3.74504	-0.49974
C	2.94747	-3.27912	-1.05967
H	2.82998	-2.95121	-2.10306
H	2.84653	-4.38340	-1.04790
H	3.96065	-3.02624	-0.70799
C	2.39506	-0.66135	-0.19963
C	3.00467	-0.37959	-1.44958
C	3.06922	-0.27367	0.98623
C	4.25196	0.25958	-1.51138
H	2.50725	-0.67575	-2.38060
C	4.31872	0.36245	0.92264
H	2.62078	-0.47537	1.96571
C	4.91769	0.61761	-0.32536
H	4.70998	0.46701	-2.48468
H	4.83206	0.64785	1.84778
H	5.90459	1.09038	-0.37236
O	-1.47743	2.69889	1.53882
H	0.06648	2.90230	2.92315
H	1.75829	2.35726	1.26442
C	1.10040	3.68075	-0.35071
C	1.94568	4.84124	0.22794
H	1.40576	5.42421	0.99635
H	2.21590	5.54511	-0.57881
H	2.88558	4.47165	0.67799
C	1.91977	2.96988	-1.44509
H	1.35627	2.13349	-1.89307

H	2.86591	2.56887	-1.04358	H	-4.30716	-2.87156	-0.92183
H	2.16859	3.68360	-2.25078	C	-2.84620	1.24880	-0.62182
C	-0.19773	4.23820	-0.97779	C	-3.97081	2.01753	-0.94380
H	-0.81849	4.79908	-0.25629	N	-1.68281	1.80119	-0.14608
H	-0.81485	3.43427	-1.41826	C	-3.91815	3.40625	-0.75179
H	0.05801	4.93553	-1.79475	H	-4.86471	1.51959	-1.32882
H	0.62990	-1.72765	2.19501	C	-1.64301	3.14140	0.04043
H	0.97674	-3.13829	3.22653	C	-2.73920	3.96923	-0.24639
H	2.16885	-4.24528	1.29313	H	-4.78364	4.03231	-0.98905
H	2.96233	-2.73606	1.73502	H	-0.69894	3.54033	0.41707
H	-1.37025	-3.21522	2.10478	H	-2.65156	5.04534	-0.07130
H	-0.36339	-4.62576	1.77206	Pd	-0.15058	0.45517	0.18147
O	-5.87406	0.63521	-0.01167	C	3.41242	-2.05274	0.28208
C	-6.90675	-0.17655	-0.61316	C	2.33185	-1.18386	-0.17549
H	-7.85158	0.31172	-0.33971	C	3.41933	-1.08161	-2.30955
H	-6.79955	-0.19595	-1.71212	C	4.76727	-1.24912	-1.61724
H	-6.88414	-1.20333	-0.20709	C	4.61468	-2.07444	-0.35726
				H	3.23893	-2.58057	1.22388

Complex 12 for TS7

E(Solv):	-1395.052749			H	3.06768	-2.04155	-2.72976
Correction to H:	0.508760			H	3.44086	-0.32359	-3.10497
Correction to G:	0.413230			H	5.47310	-1.72844	-2.32055
C	-2.81999	-0.21538	-0.72349	H	5.20700	-0.26431	-1.35817
C	-3.46396	-2.27759	-1.30161	O	1.35174	-0.93539	0.57586
C	-2.17273	-2.35019	-0.43069	C	5.80253	-2.82888	0.15910
N	-1.80559	-0.91226	-0.30034	H	5.59440	-3.33437	1.11539
				H	6.13044	-3.58629	-0.57888

H	6.66195	-2.14537	0.30105
C	1.20224	1.87819	0.54373
C	1.71412	2.02342	1.84826
C	1.64822	2.73481	-0.48357
C	2.65297	3.03663	2.12523
H	1.38618	1.35556	2.65353
C	2.59284	3.74068	-0.19902
H	1.26613	2.62513	-1.50565
C	3.09299	3.89473	1.10429
H	3.03827	3.15021	3.14524
H	2.93495	4.40337	-1.00285
H	3.82337	4.68105	1.32374
O	-3.87682	-0.86257	-1.24534
H	-1.36269	-2.86573	-0.97783
H	-3.29025	-2.51711	-2.36383
C	-2.34987	-3.06669	0.95286
C	-1.01935	-3.00485	1.73328
H	-0.19419	-3.46657	1.16063
H	-0.73151	-1.96545	1.96451
H	-1.11512	-3.55399	2.68703
C	-2.69955	-4.54847	0.67645
H	-2.78229	-5.09869	1.63003
H	-3.66355	-4.66895	0.14936
H	-1.91616	-5.04299	0.07234
C	-3.46526	-2.40380	1.79080
H	-3.22265	-1.35160	2.02529
H	-4.44960	-2.43044	1.28811
H	-3.57944	-2.93697	2.75087
O	2.37953	-0.60991	-1.38625

7-TS-A

E(Solv): -1395.024776

Correction to H: 0.507408

Correction to G: 0.419690

C	-1.93108	1.48633	-0.63885
C	-3.89776	0.52208	-1.07966
C	-3.04626	-0.42560	-0.19417
N	-1.71931	0.26610	-0.22380
H	-3.95475	0.20409	-2.13422
H	-2.93243	-1.41826	-0.66056
C	-0.87907	2.51051	-0.60520
C	-1.09892	3.85417	-0.93310
N	0.32917	2.03845	-0.17510
C	-0.03498	4.75851	-0.78922
H	-2.08489	4.17087	-1.28361
C	1.34348	2.91548	-0.03560
C	1.19867	4.28286	-0.32528
H	-0.17192	5.81678	-1.03191
H	2.29192	2.50066	0.31517
H	2.05076	4.95461	-0.18740
Pd	0.35682	-0.12645	0.05678
C	0.37103	-2.21250	0.14114

C	-0.45953	-2.71251	-1.01257	H	-3.02948	-1.69744	3.07964
C	1.40142	-2.10700	-2.41634	H	-2.40313	-2.44247	1.57761
C	2.34957	-2.59438	-1.32646	C	-3.83094	0.71810	1.98391
C	1.81919	-2.27987	0.06289	H	-2.89190	1.29118	2.09503
H	-0.08593	-2.47550	1.10569	H	-4.56925	1.35817	1.46758
O	-1.58974	-3.15903	-0.85441	H	-4.22076	0.53380	3.00044
C	2.57373	-2.92417	1.21128	C	-4.93293	-1.40436	1.14459
H	2.16020	-2.64907	2.19349	H	-4.78926	-2.37742	0.64155
H	2.45864	-4.02145	1.10099	H	-5.33975	-1.60235	2.15185
H	3.64944	-2.68859	1.18846	H	-5.70644	-0.84215	0.59015
C	2.40799	-0.23464	0.42400	H	1.29032	-1.00291	-2.38827
C	2.68004	0.00754	1.79590	H	1.73564	-2.40748	-3.42067
C	3.34566	0.20531	-0.54180	H	3.37269	-2.21434	-1.48041
C	3.84009	0.69671	2.18412	H	2.41604	-3.70117	-1.38659
H	1.98159	-0.33736	2.56741	O	0.08613	-2.70036	-2.26383
C	4.52064	0.86801	-0.14800				
H	3.16088	0.04890	-1.61000	**7-TS-B**			
C	4.76987	1.11460	1.21404	E(Solv):	-1395.021649		
H	4.02717	0.88954	3.24617	Correction to H:	0.507228		
H	5.23940	1.19431	-0.90789	Correction to G:	0.419407		
H	5.68978	1.62407	1.51994	C	-1.79554	1.69012	-0.59832
O	-3.15884	1.80682	-1.06542	C	-3.69358	0.90236	-1.46818
H	-4.90547	0.73229	-0.69675	C	-3.01882	-0.20147	-0.61880
C	-3.59886	-0.62817	1.26281	N	-1.66481	0.40408	-0.40285
C	-2.60643	-1.48169	2.08235	H	-4.75003	1.08819	-1.23430
H	-1.65002	-0.94808	2.23208	C	-0.73866	2.63991	-0.22378

C	-0.89147	4.03102	-0.27595	C	4.24552	0.36625	1.54383
N	0.39646	2.03445	0.23820	H	2.50698	-0.78652	2.10128
C	0.15973	4.83437	0.19386	C	4.93004	1.03108	0.51032
H	-1.81731	4.45992	-0.66863	H	4.91356	1.57873	-1.59472
C	1.40282	2.81390	0.68101	H	4.66195	0.34566	2.55704
C	1.31685	4.21648	0.68718	H	5.88811	1.52094	0.71427
H	0.07209	5.92508	0.17593	O	-2.95070	2.13667	-1.10845
H	2.29357	2.28951	1.03880	H	-3.56497	0.76430	-2.55544
H	2.15432	4.80524	1.07229	H	-2.90000	-1.14378	-1.17883
Pd	0.39850	-0.10347	-0.18456	C	-3.76861	-0.50811	0.73286
C	0.45791	-2.01034	-1.02544	C	-5.10803	-1.19307	0.36640
C	-0.61438	-2.88779	-0.44494	H	-5.78818	-0.53121	-0.20044
C	0.80649	-3.06822	1.48259	H	-5.63925	-1.48667	1.28872
C	2.02757	-3.11213	0.57051	H	-4.93992	-2.10791	-0.22991
C	1.84666	-2.23021	-0.65582	C	-2.94151	-1.48460	1.59482
H	0.25859	-1.80791	-2.09030	H	-1.95134	-1.06241	1.84658
O	-1.65706	-3.11945	-1.04547	H	-2.79379	-2.44880	1.08267
C	2.85727	-2.45137	-1.76670	H	-3.47107	-1.68121	2.54419
H	2.68783	-1.79011	-2.63003	C	-4.03883	0.77694	1.54806
H	2.72251	-3.49283	-2.12221	H	-4.65328	1.51466	1.00148
H	3.89570	-2.34042	-1.41690	H	-3.09962	1.26937	1.86125
C	2.47140	-0.27128	-0.02475	H	-4.58908	0.51802	2.46976
C	3.17545	0.40263	-1.05630	H	2.14439	-4.14893	0.19109
C	3.02648	-0.28180	1.27955	H	2.95359	-2.87820	1.12095
C	4.38687	1.05786	-0.78756	H	0.63927	-2.04993	1.88974
H	2.77268	0.42201	-2.07530	H	0.89231	-3.77630	2.32022

O	-0.38747	-3.47396	0.76598	C	3.44977	-1.12845	1.08921
				C	3.00868	-0.55690	-0.24628
7-TS-C				H	2.72402	1.42704	-1.10161
E(Solv):	-1395.020276			O	2.99715	2.85126	1.00950
Correction to H:	0.507257			C	3.79959	-1.02266	-1.45261
Correction to G:	0.418601			H	3.42463	-0.59290	-2.39390
C	-2.24267	0.92264	-0.58039	H	4.84019	-0.66355	-1.31747
C	-3.70661	-0.72763	-0.92637	H	3.82570	-2.12055	-1.53621
C	-2.53324	-1.24682	-0.05352	C	1.14177	-1.60367	-0.68729
N	-1.56525	-0.11394	-0.16784	C	0.96786	-1.76414	-2.08654
H	-3.65966	-1.07018	-1.97409	C	0.99059	-2.73016	0.15140
H	-2.07451	-2.14891	-0.49341	C	0.61062	-3.01070	-2.62262
C	-1.65613	2.26733	-0.61983	H	1.11089	-0.91239	-2.76224
C	-2.38796	3.40876	-0.96696	C	0.65729	-3.98337	-0.39136
N	-0.33674	2.30917	-0.25319	H	1.11807	-2.63988	1.23474
C	-1.74443	4.65573	-0.92320	C	0.46420	-4.12539	-1.77630
H	-3.43674	3.30849	-1.25920	H	0.46935	-3.11657	-3.70390
C	0.27522	3.51269	-0.21707	H	0.55020	-4.84927	0.27158
C	-0.39956	4.70429	-0.53816	H	0.21497	-5.10500	-2.19778
H	-2.28824	5.56885	-1.18421	O	-3.51948	0.73918	-0.95001
H	1.32844	3.51437	0.08973	H	-4.70818	-0.91439	-0.51649
H	0.14277	5.65240	-0.48044	C	-2.93413	-1.55795	1.43551
Pd	0.54103	0.32420	-0.15844	C	-1.68085	-1.94336	2.24873
C	2.57334	0.82571	-0.19181	H	-0.94133	-1.12272	2.26354
C	2.85143	1.63353	1.05018	H	-1.96283	-2.16624	3.29312
C	2.74552	-0.44477	2.25480	H	-1.19715	-2.84285	1.83001

C	-3.61849	-0.34596	2.10704
H	-2.94256	0.52658	2.16116
H	-4.54422	-0.03769	1.58944
H	-3.89902	-0.60480	3.14303
C	-3.90008	-2.76783	1.41966
H	-3.44292	-3.64487	0.92535
H	-4.14873	-3.05989	2.45498
H	-4.85522	-2.54767	0.90978
H	3.12331	-0.78881	3.22906
H	1.64911	-0.61000	2.21376
H	3.33287	-2.22350	1.13060
H	4.53947	-0.92837	1.16676
O	2.99024	0.98556	2.23956

7-TS-D

E(Solv): -1395.019775

Correction to H: 0.507100

Correction to G: 0.418342

C	1.43618	1.84486	0.64545
C	3.19407	1.09572	1.79905
C	2.74617	0.02309	0.77300
N	1.43389	0.58023	0.31834
H	4.26110	1.35286	1.76255
C	0.40408	2.77266	0.16900
C	0.51568	4.16273	0.28761
N	-0.64135	2.15848	-0.46625
C	-0.46887	4.96596	-0.30981
H	1.36489	4.59172	0.82619
C	-1.57876	2.94000	-1.04334
C	-1.51862	4.34392	-0.99534
H	-0.41036	6.05659	-0.24137
H	-2.42148	2.42766	-1.51434
H	-2.30543	4.92558	-1.48380
Pd	-0.57159	-0.00192	-0.29000
C	-2.57622	-0.47775	-0.68432
C	-3.45506	0.51828	0.02879
C	-2.82316	-0.61869	2.04788
C	-2.94507	-1.94351	1.30529
C	-2.48784	-1.82333	-0.13971
H	-2.70022	-0.39956	-1.77619
O	-4.06840	1.38820	-0.57796
C	-2.86002	-2.99786	-1.02501
H	-2.51885	-2.87226	-2.06299
H	-3.96791	-3.04562	-1.04645
H	-2.48558	-3.95484	-0.62791
C	-0.34884	-2.06160	-0.09920
C	0.04469	-2.72259	-1.29102
C	0.07533	-2.59622	1.14444
C	0.83340	-3.88195	-1.24087
H	-0.27564	-2.33668	-2.26583
C	0.86359	-3.75629	1.19250
H	-0.20897	-2.10746	2.08372

C	1.23308	-4.40781	0.00067
H	1.12699	-4.38060	-2.17100
H	1.17935	-4.16001	2.16100
H	1.82621	-5.32762	0.04117
O	2.44457	2.30589	1.40235
H	2.89910	0.86545	2.83730
H	2.56604	-0.95142	1.25884
C	3.76261	-0.18860	-0.40716
C	5.03707	-0.83738	0.18555
H	5.55153	-0.18531	0.91486
H	5.75926	-1.04863	-0.62241
H	4.80768	-1.79586	0.68670
C	3.15749	-1.14821	-1.44990
H	2.24673	-0.72525	-1.90792
H	2.89464	-2.11991	-0.99811
H	3.88815	-1.33610	-2.25687
C	4.12471	1.14393	-1.10149
H	4.60562	1.86867	-0.42044
H	3.23733	1.62434	-1.55258
H	4.83834	0.94979	-1.92135
H	-1.76510	-0.28483	2.09895
H	-3.23413	-0.67225	3.06700
H	-4.01724	-2.22913	1.26931
H	-2.42659	-2.75779	1.83725
O	-3.59672	0.41213	1.38159

Complex 12 for TS8

E(Solv): -1437.750544

Correction to H: 0.589440

Correction to G: 0.488111

C	2.92161	-0.26341	0.81134
C	3.41700	-2.34453	1.46145
C	2.16898	-2.36338	0.52937
N	1.88192	-0.90962	0.36826
H	4.23926	-2.99938	1.14025
C	3.04522	1.19168	0.66423
C	4.20511	1.89796	1.00357
N	1.94145	1.79753	0.11731
C	4.25463	3.27734	0.75168
H	5.04707	1.35944	1.44670
C	2.00216	3.12680	-0.13030
C	3.13941	3.89286	0.16893
H	5.14981	3.85507	1.00110
H	1.10460	3.57019	-0.56641
H	3.13316	4.96287	-0.05776
Pd	0.32840	0.53980	-0.21004
C	-2.50645	-0.33937	1.36767
C	-2.29872	-0.94995	0.07003
C	-3.34661	-1.91381	-0.49959
C	-4.74272	-1.46519	0.00824
C	-4.81613	-1.29103	1.53290
C	-3.66022	-0.49709	2.08885

H	-1.67340	0.25738	1.76121	H	0.22732	-3.37954	-1.17502
H	-4.99893	-0.50183	-0.47310	H	0.88972	-1.90939	-1.94088
H	-5.49715	-2.19943	-0.32832	H	1.22913	-3.51718	-2.64560
H	-5.76865	-0.80845	1.82383	C	2.62922	-4.59587	-0.53944
H	-4.82844	-2.27689	2.04583	H	2.73591	-5.15597	-1.48488
O	-1.23516	-0.76705	-0.60119	H	3.55193	-4.76853	0.04393
C	-3.82267	0.10088	3.45603	H	1.78450	-5.04044	0.01894
H	-2.90110	0.58238	3.82046	C	3.58303	-2.50911	-1.61561
H	-4.63469	0.85392	3.44771	H	3.42098	-1.44513	-1.86544
H	-4.13258	-0.67243	4.18506	H	4.53463	-2.59523	-1.05982
C	-0.92451	2.02823	-0.66747	H	3.71605	-3.05291	-2.56724
C	-1.46317	2.08773	-1.96867	C	-3.32281	-1.90727	-2.04166
C	-1.27573	3.01559	0.27682	H	-2.34110	-2.22137	-2.43051
C	-2.32950	3.13936	-2.32526	H	-4.08811	-2.60404	-2.42639
H	-1.20900	1.32231	-2.71135	H	-3.54313	-0.90134	-2.43979
C	-2.15150	4.05867	-0.08441	C	-2.99716	-3.33873	0.02061
H	-0.87014	2.98386	1.29577	H	-3.75496	-4.05637	-0.34094
C	-2.67594	4.12369	-1.38519	H	-2.01364	-3.66078	-0.36253
H	-2.73234	3.18421	-3.34383	H	-2.96904	-3.39355	1.12299
H	-2.42045	4.81955	0.65777				
H	-3.35226	4.93835	-1.66563	**8-TS-A**			
O	3.91832	-0.95869	1.38645	E(Solv):	-1437.720776		
H	1.30847	-2.83464	1.03727	Correction to H:	0.588142		
H	3.17745	-2.54059	2.51993	Correction to G:	0.493744		
C	2.38370	-3.09799	-0.84017	C	-1.98342	1.49112	-0.76165
C	1.10781	-2.96310	-1.69772	C	-3.94083	0.42655	-0.92175

C	-3.04064	-0.29991	0.11173	H	3.72864	-2.03291	1.90414
N	-1.73179	0.38726	-0.11098	C	2.40404	0.13463	0.61609
H	-4.02636	-0.10658	-1.88361	C	2.60733	0.68164	1.91098
H	-2.91814	-1.36763	-0.13409	C	3.35696	0.41516	-0.39436
C	-0.95560	2.51730	-0.97553	C	3.71293	1.50490	2.17657
C	-1.21546	3.75619	-1.57512	H	1.89728	0.46669	2.71818
N	0.27262	2.16896	-0.48769	C	4.47917	1.21411	-0.11710
C	-0.17105	4.69048	-1.65544	H	3.22608	0.01842	-1.40645
H	-2.21660	3.97270	-1.95745	C	4.65895	1.76049	1.16663
C	1.26784	3.07519	-0.56608	H	3.84626	1.92969	3.17750
C	1.08388	4.34657	-1.13578	H	5.21211	1.41157	-0.90738
H	-0.33918	5.67049	-2.11253	H	5.53793	2.37735	1.38207
H	2.23480	2.76308	-0.16302	O	-3.23189	1.69631	-1.20308
H	1.92285	5.04768	-1.16698	H	-4.93993	0.69590	-0.55348
Pd	0.35943	0.09856	0.19756	C	-3.54354	-0.19562	1.59717
C	0.46852	-1.92829	0.71869	C	-2.51114	-0.84764	2.54270
C	-0.34452	-2.64643	-0.32806	H	-1.56346	-0.27863	2.55468
C	0.28209	-2.98961	-1.69572	H	-2.90477	-0.86657	3.57472
C	1.66961	-2.31868	-1.84174	H	-2.29488	-1.88522	2.23378
C	2.54695	-2.50258	-0.59843	C	-3.77729	1.26959	2.02672
C	1.92328	-1.94046	0.67200	H	-2.84500	1.86179	1.97941
H	0.00949	-1.99442	1.71804	H	-4.54403	1.77858	1.41465
O	-1.49875	-3.00074	-0.05437	H	-4.12916	1.29882	3.07298
C	2.66129	-2.30205	1.95140	C	-4.86669	-0.99392	1.69156
H	2.20918	-1.84721	2.84592	H	-4.72304	-2.04889	1.39534
H	2.58967	-3.40207	2.06935	H	-5.23474	-0.98412	2.73263

H	-5.66926	-0.56710	1.06248	C	-0.62243	-5.05365	-0.41734
C	-0.66697	-2.50145	-2.81448	H	-2.48775	-4.44210	0.55212
H	-0.26538	-2.78477	-3.80371	C	0.88335	-3.21158	-0.87110
H	-1.66501	-2.95472	-2.69868	C	0.59071	-4.58437	-0.93908
H	-0.77560	-1.40085	-2.79282	H	-0.86832	-6.11971	-0.44488
C	0.39036	-4.53767	-1.76899	H	1.82615	-2.80405	-1.24672
H	0.78311	-4.83835	-2.75665	H	1.31480	-5.26706	-1.39291
H	1.05855	-4.95620	-0.99513	Pd	0.34923	-0.22682	0.17936
H	-0.60425	-4.99228	-1.63105	C	0.71310	1.61612	1.09784
H	1.52127	-1.23396	-2.02874	C	-0.03753	2.75408	0.44987
H	2.18284	-2.72652	-2.73223	C	0.69492	3.67487	-0.54700
H	3.56594	-2.10655	-0.74159	C	1.95128	2.96212	-1.09993
H	2.68221	-3.58673	-0.39952	C	2.86455	2.41393	0.00177
				C	2.16175	1.47700	0.98269
8-TS-B				H	0.29212	1.38804	2.09414
E(Solv):	-1437.714295			O	-1.19168	2.99455	0.82374
Correction to H:	0.588215			C	2.91581	1.27193	2.28961
Correction to G:	0.494316			H	2.41459	0.55913	2.96340
C	-2.06515	-1.70197	0.58947	H	2.93271	2.25063	2.80883
C	-3.78291	-0.68555	1.58606	H	3.95817	0.95434	2.12773
C	-3.02275	0.32976	0.70167	C	2.42990	-0.41049	0.08368
N	-1.77400	-0.44146	0.39863	C	2.98246	-1.34416	0.99963
H	-4.86802	-0.72286	1.42317	C	2.97191	-0.35542	-1.22760
C	-1.17069	-2.77717	0.14030	C	4.03885	-2.18671	0.62116
C	-1.52458	-4.13226	0.13780	H	2.58575	-1.41723	2.01765
N	0.02277	-2.31919	-0.34243	C	4.02845	-1.20124	-1.60499

H	2.57173	0.34997	-1.96262	H	1.62729	5.65223	-0.39222
C	4.57130	-2.11057	-0.67877	H	0.15374	5.45753	0.60816
H	4.45258	-2.89682	1.34566	H	1.69308	4.74326	1.14516
H	4.43370	-1.14091	-2.62114	H	3.23086	3.25994	0.62016
H	5.40931	-2.75396	-0.96760	H	3.77135	1.94126	-0.41023
O	-3.23936	-2.00042	1.16365	H	1.62126	2.14283	-1.76890
H	-3.56523	-0.58643	2.66362	H	2.52197	3.66719	-1.73288
H	-2.74303	1.24534	1.24740				
C	-3.80995	0.73794	-0.60078	**8-TS-C**			
C	-5.00890	1.61089	-0.15610	E(Solv):	-1437.717102		
H	-5.72365	1.06348	0.48542	Correction to H:	0.587914		
H	-5.56957	1.95249	-1.04404	Correction to G:	0.492634		
H	-4.67021	2.50765	0.39325	C	-2.29856	1.32573	-0.41524
C	-2.90656	1.57837	-1.52507	C	-4.10434	0.01241	-0.39582
H	-2.01925	1.00635	-1.85214	C	-2.92616	-0.71080	0.31057
H	-2.56377	2.49210	-1.01496	N	-1.78445	0.18867	-0.03500
H	-3.46902	1.87545	-2.42843	H	-4.31242	-0.37453	-1.40786
C	-4.32110	-0.49279	-1.38517	H	-2.73984	-1.70281	-0.13567
H	-5.02071	-1.11859	-0.80276	C	-1.46804	2.50843	-0.66861
H	-3.49000	-1.13231	-1.73561	C	-2.00392	3.75613	-1.00913
H	-4.86441	-0.15254	-2.28422	N	-0.12392	2.28716	-0.52347
C	-0.23641	4.08092	-1.70742	C	-1.12446	4.83312	-1.20151
H	-1.16242	4.53829	-1.32372	H	-3.08636	3.86603	-1.11701
H	0.27244	4.81743	-2.35441	C	0.71482	3.32748	-0.71774
H	-0.51011	3.21165	-2.33094	C	0.24960	4.61257	-1.04983
C	1.06969	4.95390	0.25757	H	-1.51008	5.82280	-1.46524

H	1.78415	3.11489	-0.58977	O	-3.63107	1.40299	-0.56131
H	0.97435	5.42056	-1.18545	H	-5.03574	0.05959	0.18429
Pd	0.34269	0.16564	-0.39153	C	-3.12042	-0.88657	1.86095
C	2.40182	0.18522	-0.79633	C	-1.85404	-1.51216	2.48248
C	3.00813	0.94466	0.35448	H	-0.96635	-0.87380	2.32590
C	3.29609	0.23848	1.69324	H	-1.99311	-1.64026	3.57071
C	2.70766	-1.19339	1.68673	H	-1.64796	-2.50612	2.04892
C	3.02278	-1.95404	0.39439	C	-3.41205	0.46229	2.55658
C	2.49564	-1.26418	-0.85388	H	-2.56779	1.16745	2.45075
H	2.50966	0.72119	-1.75440	H	-4.32473	0.95207	2.17268
O	3.32102	2.13316	0.19105	H	-3.56512	0.29740	3.63761
C	2.93613	-1.88957	-2.16572	C	-4.30512	-1.85895	2.07887
H	2.49453	-1.39203	-3.04269	H	-4.13468	-2.82544	1.56963
H	4.03574	-1.76332	-2.23395	H	-4.42536	-2.06614	3.15668
H	2.71423	-2.96780	-2.20716	H	-5.26693	-1.44917	1.72114
C	0.41548	-1.85424	-0.92197	C	2.66512	1.07112	2.83401
C	-0.05336	-1.95887	-2.25809	H	3.06698	2.09735	2.83111
C	0.16157	-2.91822	-0.02814	H	1.56563	1.12774	2.72702
C	-0.78844	-3.07998	-2.67245	H	2.89087	0.60660	3.81052
H	0.15734	-1.16146	-2.98069	C	4.83829	0.21773	1.87740
C	-0.55242	-4.05192	-0.45350	H	5.08997	-0.22215	2.85877
H	0.51455	-2.87093	1.00640	H	5.35311	-0.37175	1.09762
C	-1.03146	-4.13385	-1.77232	H	5.23705	1.24449	1.83869
H	-1.15059	-3.14103	-3.70471	H	3.08863	-1.75210	2.56141
H	-0.73191	-4.87309	0.24959	H	1.60614	-1.12274	1.80809
H	-1.57945	-5.02259	-2.10309	H	2.68521	-3.00306	0.43165

H	4.12364	-2.00724	0.25367	C	-2.46486	-2.36304	1.04934
				C	-1.97878	-2.15021	-0.37816

8-TS-D

E(Solv):	-1437.715983			H	-2.27185	-0.77965	-2.04869
Correction to H:	0.588050			O	-3.77872	0.94149	-0.98432
Correction to G:	0.493505			C	-2.16743	-3.35826	-1.28201
C	1.38817	2.00133	0.59779	H	-1.79144	-3.19291	-2.30247
C	3.01980	1.49583	2.03300	H	-3.25907	-3.53805	-1.35772
C	2.83992	0.33981	1.01572	H	-1.70217	-4.26495	-0.86261
N	1.56016	0.73150	0.34639	C	0.14191	-2.12529	-0.25827
H	4.04915	1.86305	2.14059	C	0.66952	-2.67681	-1.45552
C	0.34340	2.78750	-0.06843	C	0.58919	-2.64562	0.98269
C	0.32166	4.18720	-0.06782	C	1.60423	-3.72168	-1.41315
N	-0.56420	2.02759	-0.75430	H	0.33235	-2.30023	-2.42850
C	-0.64722	4.84022	-0.84648	C	1.52100	-3.69444	1.02273
H	1.06096	4.73844	0.51950	H	0.20166	-2.23730	1.92308
C	-1.48840	2.66454	-1.50400	C	2.01895	-4.24271	-0.17435
C	-1.55094	4.06666	-1.58474	H	1.99828	-4.13831	-2.34647
H	-0.68834	5.93343	-0.87638	H	1.84969	-4.09365	1.98884
H	-2.22535	2.03185	-2.00616	H	2.72585	-5.07866	-0.14071
H	-2.31717	4.52963	-2.21298	O	2.22349	2.60190	1.46171
Pd	-0.30150	-0.09971	-0.44580	H	2.59340	1.27888	3.02765
C	-2.20849	-0.82908	-0.94790	H	2.68995	-0.62802	1.52454
C	-3.19012	0.10542	-0.28725	C	4.03648	0.19247	0.00766
C	-3.49273	-0.02786	1.21981	C	5.26872	-0.28616	0.81253
C	-2.54864	-1.07064	1.86696	H	5.59367	0.44426	1.57599
				H	6.12305	-0.44027	0.13035

H	5.07028	-1.24723	1.32186
C	3.69481	-0.87229	-1.05279
H	2.82000	-0.57833	-1.65760
H	3.47492	-1.84774	-0.58646
H	4.55104	-1.01054	-1.73716
C	4.35744	1.52716	-0.70261
H	4.64577	2.33019	-0.00098
H	3.50337	1.88241	-1.30745
H	5.20647	1.38261	-1.39346
C	-3.30600	1.35408	1.88786
H	-2.25686	1.69493	1.81377
H	-3.95175	2.10620	1.40595
H	-3.57186	1.29575	2.95835
C	-4.98221	-0.44885	1.35286
H	-5.19014	-1.43550	0.90177
H	-5.26377	-0.49663	2.41981
H	-5.62839	0.28955	0.85068
H	-1.53256	-0.62875	1.95671
H	-2.89167	-1.29175	2.89467
H	-3.47980	-2.80232	0.95077
H	-1.86462	-3.13998	1.55104

Complex 12 for TS9

E(Solv): -1511.78109

Correction to H: 0.571732

Correction to G: 0.466387

C	3.01523	-1.24970	-0.62629
C	4.75534	0.12415	-0.92142
C	3.63356	0.85576	-0.12262
N	2.51714	-0.13018	-0.18625
H	5.73603	0.11084	-0.42571
C	2.21585	-2.47937	-0.68428
C	2.74995	-3.72232	-1.04332
N	0.90329	-2.31492	-0.31775
C	1.91848	-4.85193	-1.00588
H	3.80116	-3.78636	-1.33676
C	0.11091	-3.41142	-0.27778
C	0.58462	-4.68996	-0.61015
H	2.30894	-5.83746	-1.27697
H	-0.92607	-3.23960	0.01747
H	-0.10108	-5.54038	-0.55638
Pd	0.34844	-0.35933	0.07598
C	-1.06580	3.73967	0.29390
C	-0.72452	2.44483	-0.25616
C	-1.10205	2.12140	-1.68275
C	-1.21982	3.38679	-2.55049
C	-2.12047	4.43595	-1.87592
C	-1.74916	4.68210	-0.43122
H	-0.37062	1.39577	-2.08450
H	-0.80284	3.91544	1.34302
H	-0.21359	3.82075	-2.70447
H	-1.61402	3.12597	-3.54746

H	-2.09832	5.39099	-2.43301	C	5.17689	2.27977	1.26373
H	-3.18222	4.10639	-1.90065	H	5.44025	2.62701	2.27804
H	-2.07265	1.58302	-1.64056	H	6.09666	1.85825	0.81875
O	-0.14250	1.60685	0.50369	H	4.88715	3.16814	0.67204
C	-2.18129	5.98114	0.18229	C	4.46333	0.01734	2.16039
H	-1.94131	6.04439	1.25548	H	3.64223	-0.71542	2.25931
H	-1.69904	6.83030	-0.34034	H	5.33610	-0.49625	1.71729
H	-3.27148	6.12559	0.05307	H	4.75425	0.32577	3.17979
C	-1.59481	-0.78719	0.23597	C	-5.81747	-1.73927	0.59083
C	-2.23340	-0.63653	1.48393	O	-6.41687	-2.10910	-0.42099
C	-2.34392	-1.23550	-0.87702	C	-6.53095	-1.62082	1.93129
C	-3.59835	-0.94816	1.62092	H	-6.06165	-2.27044	2.69326
H	-1.67362	-0.27851	2.35584	H	-6.49042	-0.58483	2.31630
C	-3.70711	-1.53142	-0.73495	H	-7.58213	-1.91665	1.80088
H	-1.86639	-1.35781	-1.85732				
C	-4.35044	-1.39582	0.51444	**9-TS-A**			
H	-4.07136	-0.83562	2.60282	E(Solv):	-1511.745387		
H	-4.30652	-1.87528	-1.58534	Correction to H:	0.570507		
O	4.30243	-1.27776	-1.00947	Correction to G:	0.472998		
H	3.31586	1.77405	-0.64888	C	-2.24385	1.73387	-0.60304
H	4.86721	0.48848	-1.95604	C	-4.41114	1.19019	-0.59782
C	4.02234	1.25213	1.34430	C	-3.61333	0.13797	0.21629
C	2.81299	1.91912	2.03346	N	-2.20664	0.52436	-0.11218
H	2.46711	2.80511	1.47034	H	-4.73310	0.82813	-1.58881
H	1.96179	1.22434	2.12904	H	-3.78928	-0.88363	-0.15949
H	3.09523	2.25438	3.04740	C	-1.02191	2.50924	-0.84960

C	-1.02942	3.84046	-1.28472	H	1.51005	-0.71264	2.25244
N	0.12705	1.82392	-0.56904	C	3.99946	-0.10989	-0.69177
C	0.19898	4.50667	-1.41765	H	2.42232	-0.75998	-2.00794
H	-1.98096	4.33218	-1.50417	C	4.40318	0.16345	0.63502
C	1.30082	2.47480	-0.69624	H	3.76845	0.16442	2.72259
C	1.37833	3.81519	-1.11121	H	4.72545	0.06279	-1.49391
H	0.23031	5.54834	-1.75159	O	-3.44163	2.28380	-0.84205
H	2.19839	1.89589	-0.46442	H	-5.26389	1.63451	-0.06749
H	2.35724	4.29651	-1.19156	C	-3.90630	0.14899	1.75987
Pd	-0.23147	-0.28598	-0.11120	C	-2.97925	-0.86252	2.46835
C	-0.58582	-2.33386	0.14341	H	-1.92033	-0.55326	2.39611
C	-1.64290	-2.66461	-0.87913	H	-3.23922	-0.92695	3.54000
C	-1.21012	-2.92004	-2.32051	H	-3.08377	-1.86818	2.02464
C	0.25347	-2.54204	-2.59471	C	-3.70367	1.55035	2.37604
C	1.15999	-3.13862	-1.51024	H	-2.65870	1.89545	2.26946
C	0.81101	-2.67328	-0.10010	H	-4.36863	2.31301	1.93138
H	-0.94830	-2.45280	1.17626	H	-3.92795	1.51810	3.45680
O	-2.82295	-2.77716	-0.52951	C	-5.37193	-0.31063	1.95448
C	1.54949	-3.41344	1.00546	H	-5.54198	-1.31126	1.51743
H	1.30943	-3.02866	2.00837	H	-5.60409	-0.37112	3.03221
H	1.21431	-4.46950	0.96977	H	-6.10176	0.38849	1.50687
H	2.64132	-3.39762	0.85887	H	0.35451	-1.43661	-2.60170
C	1.78109	-0.79608	0.08403	H	0.56277	-2.89962	-3.59241
C	2.19715	-0.53536	1.41678	H	2.23174	-2.98461	-1.71798
C	2.70954	-0.57780	-0.96689	H	1.01783	-4.24143	-1.49481
C	3.48253	-0.04376	1.68609	H	-1.36591	-4.00246	-2.50496

H	-1.91399	-2.39769	-2.99286
C	5.81209	0.67741	0.84981
O	6.52712	0.90117	-0.12731
C	6.30284	0.90467	2.27035
H	5.67796	1.65066	2.79624
H	6.26161	-0.02964	2.86049
H	7.34092	1.26562	2.23484

9-TS-B

E(Solv): -1511.741908

Correction to H: 0.570343

Correction to G: 0.47325

C	-1.96302	1.95461	-0.56846
C	-3.96131	1.60311	-1.49542
C	-3.57513	0.38490	-0.62390
N	-2.12584	0.67285	-0.36495
H	-4.95737	2.01982	-1.29686
C	-0.73183	2.65314	-0.17644
C	-0.59288	4.04677	-0.19558
N	0.25068	1.81384	0.26694
C	0.59917	4.60337	0.29434
H	-1.40824	4.66766	-0.57636
C	1.39492	2.35749	0.72733
C	1.60059	3.74680	0.77127
H	0.73890	5.68873	0.30530
H	2.15772	1.65161	1.06872
H	2.53932	4.13867	1.17331
Pd	-0.20334	-0.27289	-0.18546
C	-0.53246	-2.17011	-1.00449
C	-1.72172	-2.79274	-0.32644
C	-1.49453	-3.55429	0.97431
C	-0.11055	-3.29264	1.58629
C	0.97685	-3.51518	0.52758
C	0.82117	-2.62474	-0.70307
H	-0.74358	-1.93607	-2.06251
O	-2.83297	-2.72607	-0.86326
C	1.68788	-3.03823	-1.88426
H	1.58354	-2.36132	-2.74577
H	1.33576	-4.03741	-2.21019
H	2.75168	-3.12409	-1.61096
C	1.80537	-0.83806	-0.17787
C	2.52156	-0.28047	-1.27029
C	2.46370	-0.93564	1.07756
C	3.83889	0.17234	-1.11286
H	2.04475	-0.19590	-2.25342
C	3.78127	-0.48904	1.22945
H	1.94341	-1.35786	1.94355
C	4.48830	0.06360	0.13723
H	4.36143	0.60325	-1.97360
H	4.29835	-0.55860	2.19280
O	-2.97603	2.64349	-1.11131
H	-3.83190	1.43196	-2.57797

H	-3.65224	-0.56600	-1.17642
C	-4.41928	0.26925	0.70135
C	-5.87101	-0.08231	0.29251
H	-6.35725	0.71696	-0.29593
H	-6.48545	-0.23308	1.19758
H	-5.90801	-1.01597	-0.29727
C	-3.87545	-0.87243	1.58496
H	-2.82316	-0.69532	1.87349
H	-3.94230	-1.83783	1.05647
H	-4.47178	-0.94218	2.51212
C	-4.40698	1.58372	1.51481
H	-4.82413	2.44086	0.95644
H	-3.38778	1.84901	1.85124
H	-5.02351	1.45889	2.42223
H	0.89071	-4.55615	0.14646
H	1.99673	-3.43673	0.93881
H	-0.06734	-2.25013	1.96416
H	0.05913	-3.95537	2.45264
H	-1.60871	-4.63091	0.73245
H	-2.31551	-3.31405	1.67176
C	5.91360	0.51672	0.37870
O	6.37822	0.46212	1.51755
C	6.73201	1.02662	-0.79627
H	6.81609	0.25805	-1.58690
H	6.26413	1.91737	-1.25587
H	7.73785	1.29247	-0.44017

9-TS-C

E(Solv): -1511.740436

Correction to H: 0.570159

Correction to G: 0.472094

C	1.20380	2.26625	-0.62420
C	-0.51352	3.68972	-0.51618
C	-0.77868	2.48117	0.42127
N	0.31704	1.55043	0.01137
H	-1.10177	3.66050	-1.44908
H	-1.74835	2.00502	0.19695
C	2.50787	1.71963	-1.01602
C	3.50096	2.48737	-1.63565
N	2.67556	0.39720	-0.70022
C	4.72829	1.87696	-1.93881
H	3.30371	3.53743	-1.86775
C	3.85643	-0.18369	-1.00250
C	4.90485	0.52687	-1.61404
H	5.52770	2.44953	-2.41925
H	3.95774	-1.24143	-0.72695
H	5.84457	0.00844	-1.82520
Pd	0.80668	-0.54770	-0.12048
C	1.31795	-2.57573	-0.26870
C	2.38781	-2.76773	0.77419
C	1.97381	-2.98722	2.22537
C	0.48037	-2.73561	2.47987

C	-0.36032	-3.45399	1.41693	H	1.46027	2.88987	2.17256
C	-0.04500	-3.01618	-0.00808	H	0.74717	4.48532	1.77670
H	1.69382	-2.72335	-1.29467	H	0.56824	3.80618	3.40723
O	3.57815	-2.80139	0.43667	C	-1.93720	3.76837	2.25177
C	-0.73294	-3.83558	-1.08733	H	-2.89553	3.29424	1.97075
H	-0.52106	-3.46496	-2.10178	H	-1.97837	3.98805	3.33299
H	-0.32703	-4.86533	-1.02169	H	-1.86985	4.73965	1.72906
H	-1.82292	-3.88905	-0.93711	H	0.19868	-3.08096	3.48988
C	-1.17332	-1.20042	-0.24413	H	0.27762	-1.64513	2.44384
C	-1.60574	-1.02134	-1.58508	H	-1.44324	-3.38910	1.61329
C	-2.11636	-1.03619	0.79783	H	-0.11911	-4.53958	1.44526
C	-2.92863	-0.65418	-1.86834	H	2.62262	-2.36448	2.86694
H	-0.90696	-1.16888	-2.41699	H	2.23326	-4.03808	2.46667
C	-3.43987	-0.68392	0.50972	C	-5.31165	-0.10805	-1.05231
H	-1.82037	-1.17543	1.84158	O	-6.04367	0.09445	-0.08298
C	-3.86400	-0.48760	-0.82298	C	-5.82350	0.01144	-2.47904
H	-3.23166	-0.51361	-2.91144	H	-5.26520	0.78103	-3.04422
H	-4.17957	-0.55226	1.30713	H	-5.70629	-0.94322	-3.02493
O	0.90612	3.54443	-0.90381	H	-6.88809	0.28553	-2.45300
H	-0.61576	4.67438	-0.04095				
C	-0.73522	2.84019	1.95179	**9-TS-D**			
C	-0.88320	1.55777	2.79687	E(Solv):	-1511.73972		
H	-0.07615	0.83568	2.57676	Correction to H:	0.569955		
H	-0.83477	1.80682	3.87180	Correction to G:	0.471922		
H	-1.85379	1.06630	2.60982	C	-1.60602	2.09149	0.63095
C	0.58537	3.54534	2.33459	C	-0.22743	3.32727	1.87761

C	0.59212	2.48848	0.86404	C	1.19359	-1.20310	-0.09361
N	-0.45206	1.55126	0.34438	C	1.92588	-1.13753	-1.30819
H	0.00062	4.40158	1.88008	C	1.88854	-0.97896	1.12550
C	-2.86092	1.57054	0.07654	C	3.30233	-0.87278	-1.30537
C	-4.06477	2.28407	0.10780	H	1.41935	-1.31135	-2.26460
N	-2.72705	0.36049	-0.54908	C	3.25975	-0.71060	1.12483
C	-5.17212	1.75679	-0.57608	H	1.35194	-1.01927	2.08025
H	-4.11433	3.23575	0.64374	C	3.98749	-0.67025	-0.08728
C	-3.79474	-0.13378	-1.21072	H	3.84095	-0.83172	-2.25801
C	-5.02685	0.54182	-1.25611	H	3.80931	-0.53788	2.05669
H	-6.12676	2.29186	-0.57952	O	-1.62407	3.18281	1.41260
H	-3.66898	-1.11806	-1.67016	H	-0.19367	2.93372	2.90811
H	-5.85656	0.09666	-1.81241	H	1.37841	1.89958	1.36630
Pd	-0.76419	-0.51410	-0.28720	C	1.25968	3.34674	-0.27172
C	-1.15728	-2.54626	-0.64561	C	2.38360	4.18686	0.38166
C	-2.45690	-2.84796	0.05363	H	2.00409	4.89811	1.13810
C	-2.44262	-3.05798	1.56544	H	2.90060	4.78381	-0.39000
C	-1.08841	-2.72531	2.21017	H	3.13911	3.54288	0.86853
C	0.04045	-3.40266	1.42434	C	1.88689	2.41626	-1.32816
C	0.09688	-2.99386	-0.04549	H	1.12153	1.80518	-1.83698
H	-1.23951	-2.65822	-1.74032	H	2.62419	1.73360	-0.87277
O	-3.49358	-2.96565	-0.60851	H	2.40785	3.01638	-2.09551
C	1.00456	-3.87864	-0.88857	C	0.23964	4.27853	-0.96434
H	1.04942	-3.56557	-1.94209	H	-0.21020	5.01424	-0.27381
H	0.57151	-4.89903	-0.86667	H	-0.57550	3.70742	-1.44470
H	2.02569	-3.93420	-0.47790	H	0.74660	4.85222	-1.75995

H	-0.93626	-1.62542	2.20923
H	-1.07228	-3.05240	3.26451
H	-0.14036	-4.49962	1.41750
H	1.02720	-3.27284	1.89882
H	-3.27351	-2.47562	2.00304
H	-2.70006	-4.12244	1.73783
C	5.47571	-0.39891	-0.00288
O	5.98340	-0.16364	1.09404
C	6.30110	-0.42395	-1.27867
H	6.22146	-1.40287	-1.78675
H	5.95416	0.34475	-1.99438
H	7.35351	-0.23053	-1.02539

Complex 12 for TS10

E(Solv): -1696.168903

Correction to H: 0.540117

Correction to G: 0.433805

C	3.15373	-1.39230	-0.62108
C	4.96275	-0.11611	-0.93762
C	3.88542	0.68272	-0.14248
N	2.71705	-0.24297	-0.19196
H	5.94412	-0.17472	-0.44666
C	2.28914	-2.57767	-0.66518
C	2.75655	-3.85364	-1.00042
N	0.98554	-2.33622	-0.30925
C	1.86485	-4.93571	-0.94814
H	3.80419	-3.97983	-1.28638
C	0.13464	-3.38741	-0.25435
C	0.54004	-4.69530	-0.56184
H	2.20265	-5.94553	-1.19989
H	-0.89243	-3.15484	0.03388
H	-0.19040	-5.50670	-0.49588
Pd	0.53970	-0.35046	0.06018
C	-0.63762	3.81958	0.31875
C	-0.37590	2.51476	-0.25033
C	-0.78275	2.23129	-1.67718
C	-0.83538	3.51260	-2.52784
C	-1.66990	4.60196	-1.83232
C	-1.27417	4.80800	-0.38787
H	-0.09712	1.47077	-2.09461
H	-0.35652	3.96631	1.36760
H	0.19263	3.89071	-2.68505
H	-1.25157	3.28755	-3.52459
H	-1.59825	5.56144	-2.37752
H	-2.74876	4.33324	-1.85237
H	-1.78200	1.74853	-1.63268
O	0.16306	1.63542	0.49459
C	-1.63072	6.11965	0.24660
H	-1.37851	6.15533	1.31822
H	-1.10898	6.94914	-0.26958
H	-2.71290	6.32270	0.12963
C	-1.42899	-0.66172	0.19827

C	-2.07294	-0.45862	1.43632	F	-6.35521	-0.08030	0.30182
C	-2.19002	-1.07492	-0.91694	F	-6.07231	-1.64167	1.81629
C	-3.45574	-0.67765	1.56007	F	-6.18116	-2.17799	-0.31571
H	-1.50320	-0.13212	2.31380				
C	-3.57534	-1.28288	-0.79398	**10-TS-A**			
H	-1.71086	-1.24199	-1.88930	E(Solv):	-1696.133776		
C	-4.20838	-1.08686	0.44553	Correction to H:	0.538907		
H	-3.94819	-0.53520	2.52728	Correction to G:	0.440575		
H	-4.16091	-1.60561	-1.66095	C	-2.36729	1.77975	-0.63318
O	4.43648	-1.49333	-1.00597	C	-4.55326	1.31944	-0.65140
H	3.61526	1.61129	-0.67712	C	-3.80817	0.24868	0.18754
H	5.08758	0.22901	-1.97732	N	-2.38329	0.57426	-0.13027
C	4.30196	1.07227	1.31862	H	-4.87280	0.95753	-1.64326
C	3.13610	1.81653	2.00398	H	-4.02268	-0.77042	-0.17469
H	2.84001	2.71512	1.43227	C	-1.11327	2.50662	-0.86580
H	2.24574	1.17464	2.11104	C	-1.06232	3.83770	-1.29842
H	3.44188	2.14623	3.01291	N	0.00362	1.77752	-0.56732
C	5.51390	2.03056	1.22323	C	0.19275	4.45718	-1.40588
H	5.79226	2.38172	2.23220	H	-1.99025	4.36593	-1.53357
H	6.40993	1.54790	0.79221	C	1.20335	2.38395	-0.66941
H	5.27912	2.92252	0.61288	C	1.33911	3.72174	-1.07757
C	4.67423	-0.17656	2.14711	H	0.26976	5.49783	-1.73553
H	3.81171	-0.85786	2.25912	H	2.07420	1.77356	-0.41839
H	5.51213	-0.74526	1.70425	H	2.33647	4.16722	-1.13394
H	4.98949	0.12568	3.16108	Pd	-0.44434	-0.31270	-0.10844
C	-5.70720	-1.25287	0.56430	C	-0.87618	-2.33884	0.18871

C	-1.95293	-2.66515	-0.81473	H	-3.51910	-0.77851	3.53181
C	-1.54302	-2.97757	-2.25115	H	-3.36343	-1.74228	2.03036
C	-0.06909	-2.66032	-2.54579	C	-3.87247	1.69997	2.32268
C	0.82295	-3.26047	-1.45104	H	-2.81535	2.00760	2.22142
C	0.50606	-2.73775	-0.05319	H	-4.50676	2.47764	1.85952
H	-1.23463	-2.41658	1.22696	H	-4.10785	1.69306	3.40155
O	-3.13255	-2.72714	-0.45198	C	-5.60126	-0.10711	1.91058
C	1.22161	-3.47537	1.06933	H	-5.80070	-1.11020	1.49203
H	1.00794	-3.04981	2.06172	H	-5.85006	-0.13609	2.98589
H	0.83974	-4.51596	1.06945	H	-6.29967	0.60758	1.43803
H	2.31176	-3.51282	0.91419	H	0.06932	-1.55948	-2.58168
C	1.55151	-0.90464	0.06493	H	0.21945	-3.05464	-3.53574
C	2.00649	-0.61547	1.37898	H	1.89828	-3.15843	-1.67138
C	2.46007	-0.74772	-1.01112	H	0.63477	-4.35521	-1.39985
C	3.30891	-0.14876	1.60455	H	-1.73963	-4.05829	-2.40338
H	1.33748	-0.74888	2.23674	H	-2.23279	-2.44890	-2.93313
C	3.77453	-0.31464	-0.78395	C	5.59394	0.54126	0.74832
H	2.14566	-0.95256	-2.03927	F	5.59992	1.89521	0.57132
C	4.19902	-0.00911	0.52311	F	6.48455	0.01310	-0.13030
H	3.64251	0.08490	2.62014	F	6.03670	0.29135	2.00610
H	4.47150	-0.21086	-1.62158				
O	-3.53942	2.37276	-0.89291	**10-TS-B**			
H	-5.39696	1.80226	-0.14031	E(Solv):	-1696.130435		
C	-4.11755	0.29614	1.72730	Correction to H:	0.53889		
C	-3.23626	-0.73538	2.46496	Correction to G:	0.441229		
H	-2.16688	-0.45999	2.41186	C	-2.11402	1.98320	-0.57831

C	-4.15567	1.68241	-1.42586	H	2.40431	-3.20937	-1.73135
C	-3.77294	0.46097	-0.55677	C	1.57068	-0.93062	-0.22345
N	-2.30799	0.70900	-0.35432	C	2.29786	-0.38382	-1.31428
H	-5.13005	2.13104	-1.19260	C	2.22919	-1.05590	1.02612
C	-0.84901	2.64758	-0.23833	C	3.62161	0.04492	-1.15655
C	-0.66087	4.03413	-0.29979	H	1.82397	-0.28396	-2.29684
N	0.11560	1.78477	0.19976	C	3.56009	-0.63919	1.18386
C	0.56607	4.55941	0.13601	H	1.70546	-1.47609	1.89036
H	-1.46476	4.67414	-0.67324	C	4.25742	-0.08772	0.09345
C	1.29169	2.29886	0.61099	H	4.16772	0.46892	-2.00510
C	1.55041	3.67990	0.60658	H	4.05885	-0.74716	2.15190
H	0.74621	5.63850	0.10953	O	-3.12516	2.69611	-1.09155
H	2.03857	1.57662	0.95179	H	-4.07444	1.49728	-2.51073
H	2.51701	4.04612	0.96415	H	-3.89710	-0.49188	-1.09737
Pd	-0.42038	-0.29330	-0.20690	C	-4.56994	0.38065	0.79988
C	-0.83408	-2.17870	-1.01398	C	-6.04579	0.07134	0.44796
C	-2.02091	-2.77681	-0.30945	C	-4.02745	-0.77143	1.67102
C	-1.77976	-3.56553	0.97223	H	-2.95761	-0.62894	1.91050
C	-0.37053	-3.35909	1.54634	H	-4.15129	-1.73885	1.15680
C	0.67899	-3.59162	0.45178	H	-4.58376	-0.81187	2.62443
C	0.51487	-2.67414	-0.75812	C	-4.48501	1.69998	1.60091
H	-1.06970	-1.93032	-2.06372	H	-4.89687	2.56537	1.05140
O	-3.14459	-2.66991	-0.81240	H	-3.44532	1.93559	1.89410
C	1.33583	-3.08870	-1.97094	H	-5.06848	1.60263	2.53333
H	1.22553	-2.39383	-2.81748	H	0.55125	-4.62214	0.05419
H	0.94639	-4.07127	-2.30451	H	1.71210	-3.55100	0.83466

H	-0.28558	-2.32742	1.94491
H	-0.19579	-4.04537	2.39316
H	-1.93751	-4.63371	0.71803
H	-2.57097	-3.30930	1.69795
C	5.66870	0.43545	0.27608
H	-6.52999	0.88359	-0.12418
H	-6.63008	-0.06002	1.37565
H	-6.13195	-0.86179	-0.13756
F	5.64275	1.77787	0.52870
F	6.41786	0.24722	-0.83987
F	6.29732	-0.16429	1.31832

10-TS-C

E(Solv): -1696.129757

Correction to H: 0.538620

Correction to G: 0.439071

C	1.31102	2.29051	-0.60898
C	-0.44362	3.66434	-0.46139
C	-0.65673	2.44451	0.47459
N	0.45706	1.54691	0.03987
H	-1.04854	3.62248	-1.38293
H	-1.61714	1.94344	0.26503
C	2.62233	1.78237	-1.02725
C	3.58244	2.58034	-1.66028
N	2.83226	0.46332	-0.72202
C	4.82053	2.00569	-1.98857
H	3.35192	3.62556	-1.88341
C	4.02326	-0.08305	-1.04791
C	5.04045	0.65960	-1.67395
H	5.59487	2.60251	-2.48041
H	4.15840	-1.13903	-0.78047
H	5.99026	0.16858	-1.90455
Pd	1.00394	-0.53426	-0.11097
C	1.56616	-2.54529	-0.29740
C	2.65844	-2.73300	0.72342
C	2.27579	-3.00311	2.17435
C	0.78153	-2.79398	2.46027
C	-0.05998	-3.50728	1.39436
C	0.21942	-3.02801	-0.02495
H	1.92880	-2.66329	-1.33197
O	3.84328	-2.72364	0.36609
C	-0.46393	-3.84108	-1.11206
H	-0.27861	-3.44256	-2.12126
H	-0.02942	-4.86053	-1.07662
H	-1.54956	-3.92832	-0.94662
C	-0.96165	-1.24339	-0.19680
C	-1.42812	-1.03942	-1.52298
C	-1.88256	-1.12591	0.86766
C	-2.75987	-0.68217	-1.76810
H	-0.74898	-1.15753	-2.37512
C	-3.22364	-0.79289	0.62213
H	-1.56288	-1.28637	1.90088

C	-3.66228	-0.56325	-0.69367	F	-5.17113	1.23598	-0.98077
H	-3.10703	-0.52088	-2.79345	F	-5.93475	-0.56659	0.01340
H	-3.93134	-0.71485	1.45333				
O	0.97220	3.56049	-0.87638	**10-TS-D**			
H	-0.56360	4.64373	0.02051	E(Solv):	-1696.12874		
C	-0.59509	2.79551	2.00623	Correction to H:	0.538497		
C	-0.69496	1.50421	2.84493	Correction to G:	0.439528		
H	0.12768	0.80564	2.60744	C	-1.64070	2.14078	0.66739
H	-0.63655	1.74707	3.92080	C	-0.15233	3.29562	1.86294
H	-1.65457	0.98738	2.66912	C	0.58283	2.43121	0.80690
C	0.71385	3.53171	2.37018	N	-0.52771	1.54588	0.33013
H	1.60154	2.89829	2.19116	H	0.12668	4.35768	1.86647
H	0.84230	4.47681	1.81262	C	-2.94250	1.69198	0.15984
H	0.70827	3.78877	3.44386	C	-4.10462	2.46683	0.24951
C	-1.81438	3.69140	2.33385	N	-2.89829	0.48590	-0.48633
H	-2.76535	3.19984	2.05760	C	-5.26504	2.00888	-0.39510
H	-1.84665	3.89559	3.41842	H	-4.08212	3.41176	0.79901
H	-1.77602	4.67073	1.82378	C	-4.01599	0.05933	-1.11159
H	0.52593	-3.16987	3.46626	C	-5.21159	0.79925	-1.09732
H	0.55415	-1.70795	2.45384	H	-6.18929	2.59330	-0.35199
H	-1.14079	-3.47358	1.60912	H	-3.96110	-0.92162	-1.59169
H	0.20745	-4.58700	1.39284	H	-6.08493	0.40726	-1.62616
H	2.92092	-2.38367	2.82269	Pd	-0.98106	-0.49590	-0.29323
H	2.56352	-4.05404	2.38072	C	-1.49611	-2.49263	-0.69541
C	-5.09020	-0.12693	-0.95456	C	-2.79049	-2.76273	0.02733
F	-5.54062	-0.58337	-2.15151	C	-2.74772	-3.03603	1.52805

C	-1.36158	-2.79855	2.14621	H	3.15672	3.42165	0.72557
C	-0.29106	-3.49779	1.29939	C	1.80852	2.33848	-1.43081
C	-0.25169	-3.02360	-0.15055	H	1.02446	1.70128	-1.87503
H	-1.61220	-2.55315	-1.79138	H	2.59681	1.68623	-1.01907
O	-3.84777	-2.80513	-0.61040	H	2.25994	2.93658	-2.24239
C	0.59979	-3.89481	-1.06138	C	0.21447	4.23369	-1.00447
H	0.63439	-3.52659	-2.09746	H	-0.20789	4.96577	-0.29299
H	0.12241	-4.89523	-1.08603	H	-0.62037	3.68296	-1.47474
H	1.62614	-4.01768	-0.67989	H	0.71269	4.81103	-1.80276
C	0.94504	-1.27330	-0.12272	H	-1.15520	-1.70816	2.18554
C	1.69222	-1.18766	-1.32533	H	-1.33342	-3.17068	3.18519
C	1.62922	-1.12462	1.11035	H	-0.53341	-4.58161	1.24556
C	3.07104	-0.94255	-1.29884	H	0.71327	-3.44622	1.75179
H	1.19544	-1.31546	-2.29350	H	-3.53556	-2.43130	2.01243
C	3.00820	-0.88018	1.13992	H	-3.05486	-4.09239	1.66522
H	1.08373	-1.19399	2.05764	C	5.19926	-0.42076	-0.03572
C	3.73025	-0.78946	-0.06549	F	5.33603	0.93943	-0.06989
H	3.63686	-0.87403	-2.23301	F	5.80699	-0.86182	1.09539
H	3.52858	-0.76790	2.09626	F	5.86818	-0.92471	-1.10279
O	-1.57235	3.22416	1.45641				
H	-0.09467	2.88849	2.88715	**Coordinates in Figure 4**			
H	1.36376	1.80382	1.26902	**Water**			
C	1.23498	3.27520	-0.34989	E(Solv):	-76.411768		
C	2.40180	4.08563	0.26572	Correction to H:	0.024338		
H	2.06828	4.80905	1.03223	Correction to G:	0.002864		
H	2.90835	4.66656	-0.52480	O	0.00000	0.00000	0.12151

H	0.00000	0.76592	-0.48604
H	0.00000	-0.76592	-0.48604

$B(OH)_3$

E(Solv): -252.466428

Correction to H: 0.052652

Correction to G: 0.020759

B	0.00000	0.00015	0.00002
O	0.01403	-1.38222	-0.00000
H	-0.90094	-1.72450	0.00017
O	1.19027	0.70332	-0.00014
H	1.94382	0.08154	0.00075
O	-1.20420	0.67885	-0.00010
H	-1.04372	1.64254	0.00094

$B(OH)_2Ph$

E(Solv): -408.240523

Correction to H: 0.130303

Correction to G: 0.088224

C	-1.95526	-1.21630	0.00007
C	-0.55251	-1.21253	0.00007
C	0.17690	-0.00001	0.00001
C	-0.55250	1.21253	-0.00006
C	-1.95524	1.21630	-0.00008
C	-2.65934	0.00000	0.00000
H	-2.50225	-2.16652	0.00011
H	-0.00536	-2.16220	0.00012
H	-0.00533	2.16219	-0.00012
H	-2.50224	2.16652	-0.00011
H	-3.75586	0.00001	-0.00000
B	1.74410	-0.00000	0.00001
O	2.39383	1.22428	0.00009
H	3.36848	1.15390	0.00050
O	2.39384	-1.22428	-0.00012
H	3.36849	-1.15390	-0.00034

Enone (2)

E(Solv): -347.976737

Correction to H: 0.160016

Correction to G: 0.119145

C	0.08921	-1.09668	-0.06294
C	-1.30156	-0.59936	0.01796
C	-1.47453	0.90492	0.25969
C	-0.32448	1.72464	-0.34950
C	1.03940	1.21410	0.14900
C	1.18318	-0.29038	0.01939
H	-2.46196	1.20660	-0.12967
H	0.19684	-2.18366	-0.16965
H	-0.35823	1.63447	-1.45259
H	-0.44130	2.79807	-0.11277
H	1.86510	1.71319	-0.39515
H	1.18227	1.49048	1.21692

H	-1.50404	1.05984	1.35922
O	-2.26946	-1.36352	-0.06529
C	2.58575	-0.84054	0.00159
H	2.59922	-1.94233	-0.03917
H	3.15046	-0.45039	-0.86800
H	3.14538	-0.51832	0.90197

Product (3)

E(Solv): -580.223165

Correction to H: 0.266815

Correction to G: 0.214454

C	1.04394	-0.88087	-0.61371
C	2.56926	-0.80307	-0.52446
C	3.14676	0.60259	-0.67723
C	2.43626	1.60163	0.26674
C	0.90321	1.52708	0.13244
C	0.32156	0.10493	0.36998
H	4.23561	0.56544	-0.50588
H	0.74496	-1.92709	-0.43553
H	2.74092	1.39745	1.31040
H	2.77608	2.62970	0.04272
H	0.44002	2.24016	0.84085
H	0.62254	1.86372	-0.88614
H	2.97831	0.92224	-1.72713
O	3.26883	-1.79593	-0.34268
C	0.58939	-0.33911	1.83317
H	1.67035	-0.39075	2.05391
H	0.12276	0.36579	2.54443
H	0.16963	-1.34059	2.02811
C	-1.19878	0.04634	0.10590
C	-1.87718	-1.19178	0.19212
C	-1.96580	1.18560	-0.21513
C	-3.25626	-1.28977	-0.03801
H	-1.32028	-2.10205	0.44339
C	-3.34987	1.09329	-0.44468
H	-1.48945	2.16769	-0.28866
C	-4.00265	-0.14399	-0.35936
H	-3.74914	-2.26615	0.03467
H	-3.91631	1.99877	-0.69153
H	-5.08096	-0.21704	-0.53973
H	0.74528	-0.61711	-1.64908

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E(Solv): -1106.350120

Correction to H: 0.308810

Correction to G: 0.235370

C	2.94608	-0.90073	0.30609
C	3.44431	-3.09548	0.40547
C	1.94433	-2.91164	0.02223
N	1.78529	-1.44209	0.03683
H	4.04638	-3.59575	-0.36654
H	1.70128	-3.29930	-0.98148

C	3.05587	0.55921	0.34478	H	-3.94301	-0.52000	3.32468
C	4.19965	1.28814	0.68120	H	-6.29360	0.03656	2.66609
N	1.86728	1.16505	0.02194	H	-1.03404	1.49736	-1.85538
C	4.11616	2.69094	0.69338	O	3.97760	-1.71192	0.53067
H	5.12527	0.76105	0.92893	H	3.59852	-3.58048	1.38061
C	1.78575	2.51179	0.04714	H	1.25746	-3.37219	0.75171
C	2.89601	3.30593	0.37825				
H	4.99266	3.29255	0.95185	**7-ts**			
H	0.80863	2.93926	-0.19510	E(Solv):	-1106.325472		
H	2.78966	4.39431	0.38592	Correction to H:	0.307037		
Pd	0.33149	-0.11068	-0.42712	Correction to G:	0.235527		
O	-1.18312	1.16057	-0.93770	C	-2.36605	0.93541	-0.13087
B	-2.28834	0.04305	-1.15934	C	-3.28216	1.98972	-0.20373
O	-1.29863	-1.22192	-0.92047	C	-2.82818	3.24025	-0.65108
H	-1.63528	-1.72123	-0.13976	C	-1.47960	3.38750	-1.00805
O	-2.59361	0.14082	-2.53162	C	-0.61105	2.28947	-0.90686
H	-3.49037	-0.17749	-2.74698	N	-1.04350	1.08502	-0.47429
C	-3.42720	0.04763	-0.04363	H	-3.51934	4.08541	-0.72153
C	-4.76242	0.37403	-0.37858	H	-4.32376	1.81964	0.08279
C	-3.16365	-0.26819	1.31359	H	-1.08771	4.34413	-1.36468
C	-5.78658	0.37013	0.57999	H	0.44938	2.35323	-1.16283
H	-5.01030	0.65415	-1.41109	C	-2.67008	-0.42795	0.29466
C	-4.17839	-0.27424	2.28302	N	-1.72275	-1.32985	0.25921
H	-2.13514	-0.49139	1.63851	C	-3.76457	-2.24939	1.04174
C	-5.49657	0.04101	1.91466	C	-2.26952	-2.60233	0.77414
H	-6.81098	0.62644	0.28824	H	-4.07273	-2.37210	2.09007

H	-1.72274	-2.89758	1.68567
Pd	0.10210	-0.59642	-0.33115
O	1.33373	-2.20466	-0.21204
B	2.48695	-1.18451	-0.88019
O	1.80899	-0.61285	-2.05997
H	1.88560	-1.20282	-2.84233
O	3.61923	-1.94813	-1.21912
H	4.25108	-2.04310	-0.48202
C	2.46049	0.00537	0.23871
C	2.26811	-0.22629	1.63768
C	2.82723	1.32886	-0.15671
C	2.44158	0.79936	2.58070
H	2.01366	-1.23592	1.97989
C	3.00330	2.35039	0.78287
H	3.00424	1.52546	-1.22061
C	2.80752	2.08722	2.15489
H	2.30314	0.59318	3.64769
H	3.31348	3.35042	0.45896
H	2.95314	2.88608	2.89055
H	1.09356	-2.87292	-0.89482
O	-3.87631	-0.80156	0.72943
H	-4.46888	-2.77119	0.37672
H	-2.14710	-3.39820	0.02081

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E(Solv): -1106.375051

Correction to H: 0.309299

Correction to G: 0.232602

C	-2.36398	-1.16906	-0.09512
C	-3.31276	-2.18333	-0.26128
C	-2.86971	-3.50645	-0.41135
C	-1.49240	-3.76019	-0.38979
C	-0.59340	-2.69547	-0.22242
N	-1.01194	-1.41643	-0.07817
H	-3.58913	-4.32053	-0.54117
H	-4.37493	-1.92406	-0.26822
H	-1.09822	-4.77435	-0.50062
H	0.48796	-2.84686	-0.20592
C	-2.71547	0.24459	0.08852
N	-1.79188	1.14593	0.24527
C	-3.97641	2.09844	0.27941
C	-2.46763	2.44321	0.45183
H	-4.43156	2.52926	-0.62602
H	-2.09582	3.17286	-0.28479
Pd	0.17389	0.24535	0.17903
O	1.41188	1.96112	0.49873
B	1.59909	3.04156	-0.40082
O	2.89557	3.45774	-0.52406
H	3.05584	4.23336	-1.09369
C	1.90186	-0.74823	0.13282
C	2.62348	-0.90906	1.33571
C	2.45324	-1.20101	-1.08385

C	3.89113	-1.52731	1.31591
H	2.19858	-0.58423	2.29459
C	3.72018	-1.81606	-1.09153
H	1.90892	-1.07241	-2.02740
C	4.43782	-1.97957	0.10533
H	4.44190	-1.65814	2.25433
H	4.14605	-2.16143	-2.04058
H	5.42217	-2.45932	0.09336
O	0.45536	3.51580	-0.98726
O	-4.00220	0.62672	0.11241
H	-4.59677	2.33200	1.15710
H	-2.22615	2.82215	1.46052
H	2.28436	1.61590	0.80462
H	0.59839	4.26129	-1.60068

9-ts

E(Solv): -1454.258951

Correction to H: 0.468858

Correction to G: 0.380530

C	-3.69770	-0.31899	0.34175
C	-4.84554	-2.23257	0.65868
C	-3.38213	-2.56200	0.23556
N	-2.79138	-1.22094	0.06832
H	-5.60351	-2.55497	-0.07051
H	-3.31404	-3.11744	-0.71405
C	-3.34787	1.09997	0.24474
C	-4.19881	2.16530	0.55258
N	-2.05076	1.28570	-0.16760
C	-3.69213	3.47172	0.45062
H	-5.22676	1.96480	0.86741
C	-1.55804	2.54068	-0.24823
C	-2.35878	3.65516	0.05937
H	-4.32991	4.32979	0.68358
H	-0.50279	2.62836	-0.54368
H	-1.92297	4.65594	-0.01190
Pd	-1.04195	-0.48061	-0.59718
C	1.98406	-1.73980	-0.97821
C	0.93771	-2.34043	-0.29785
C	1.17341	-3.04535	1.02720
C	2.28960	-2.36952	1.85655
C	3.50486	-1.93819	1.01472
C	3.18671	-1.26806	-0.32881
H	0.23044	-3.08564	1.60117
H	1.82411	-1.44792	-2.01933
H	1.87272	-1.48796	2.37309
H	2.62721	-3.05475	2.65502
H	4.18099	-1.29985	1.61153
H	4.09670	-2.83860	0.74605
H	1.44372	-4.09697	0.80047
O	-0.28870	-2.35930	-0.82446
C	4.40394	-1.16503	-1.24067
H	4.20151	-0.50562	-2.09965

H	5.29983	-0.81854	-0.69938
H	4.61829	-2.17681	-1.63393
O	0.51593	0.58580	-1.57569
B	1.88005	1.27038	-1.32738
O	1.66222	2.65705	-0.96215
H	1.40944	3.12954	-1.78413
O	2.58285	1.02321	-2.56527
H	3.26987	1.70365	-2.70327
C	2.73009	0.63935	0.10547
C	3.98002	1.33319	0.28242
C	1.84867	0.68086	1.23985
C	4.32345	1.98178	1.46843
H	4.68350	1.36962	-0.55736
C	2.15928	1.36347	2.41657
H	0.87209	0.18084	1.15589
C	3.41110	1.99853	2.54167
H	5.28834	2.49191	1.56183
H	1.44480	1.39501	3.24701
H	3.67351	2.51008	3.47450
H	0.60124	0.16435	-2.45838
O	-4.90870	-0.74703	0.70762
H	-5.11195	-2.59199	1.66341
H	-2.82188	-3.12217	1.00181

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E(Solv): -1454.351046

Correction to H: 0.472483

Correction to G: 0.379963

C	3.97512	0.84584	0.13914
C	4.41883	3.05328	0.03180
C	2.93065	2.79501	-0.35093
N	2.81312	1.33132	-0.20955
H	5.02195	3.48430	-0.78068
H	2.68502	3.08431	-1.38607
C	4.13171	-0.60054	0.32227
C	5.30598	-1.23494	0.74034
N	2.97670	-1.28689	0.04520
C	5.29235	-2.63195	0.88663
H	6.20090	-0.64083	0.94563
C	2.97013	-2.62741	0.19234
C	4.10985	-3.33366	0.61204
H	6.19280	-3.16129	1.21242
H	2.02422	-3.12615	-0.03678
H	4.05855	-4.42119	0.71668
Pd	1.37623	-0.04572	-0.54748
C	-2.29866	1.26054	-0.78960
C	-1.02816	1.49173	-0.32975
C	-0.76326	2.06792	1.05150
C	-1.97076	1.88818	1.98487
C	-3.26414	2.34371	1.28505
C	-3.58547	1.58308	-0.03392
H	0.13585	1.58036	1.47716

H	-2.40395	0.85387	-1.80357	H	-5.05790	-2.09117	2.64267
H	-2.02890	0.82347	2.27443	H	-5.96860	-3.33738	0.66250
H	-1.82385	2.46541	2.91578	H	0.01522	-1.73485	-2.00922
H	-4.13099	2.28959	1.96918	O	4.98299	1.70595	0.31161
H	-3.15143	3.41511	1.03019	H	4.54690	3.64460	0.95071
H	-0.51450	3.14464	0.94287	H	2.21571	3.29277	0.32408
O	0.02581	1.32117	-1.15305				
C	-4.48940	2.50091	-0.90666	**11**			
H	-4.73576	2.04886	-1.88210	E(Solv):	-853.873542		
H	-5.43740	2.72255	-0.38420	Correction to H:	0.254164		
H	-3.97011	3.45409	-1.10733	Correction to G:	0.379963		
O	0.04915	-1.68398	-1.02854	C	2.49087	-0.41519	0.04690
B	-1.29781	-1.78363	-0.54054	C	3.93109	-2.14248	0.16210
O	-2.21033	-2.05292	-1.51798	C	2.45989	-2.65606	0.15926
H	-3.15100	-2.03812	-1.22559	N	1.65899	-1.41605	0.05910
O	-1.42956	-1.66827	0.81054	H	4.49059	-2.38331	1.07796
H	-2.36765	-1.63753	1.10495	H	2.19109	-3.19475	1.08432
C	-4.29843	0.22067	0.19959	C	2.01089	0.97260	-0.03945
C	-4.83753	-0.49357	-0.89867	C	2.86131	2.08297	-0.07917
C	-4.39949	-0.38837	1.47202	N	0.64495	1.09675	-0.08703
C	-5.43379	-1.75805	-0.73812	C	2.29700	3.36477	-0.17712
H	-4.79643	-0.06022	-1.90362	H	3.94289	1.92870	-0.03500
C	-4.98834	-1.65833	1.63838	C	0.10464	2.33334	-0.18449
H	-4.03682	0.13373	2.36202	C	0.90260	3.48727	-0.23226
C	-5.50276	-2.35498	0.53405	H	2.93897	4.25008	-0.21161
H	-5.85919	-2.26885	-1.60968	H	-0.98533	2.38173	-0.22242

H	0.41856	4.46471	-0.31298	C	3.32500	-0.47743	0.17433
Pd	-0.38497	-0.69825	-0.00386	C	4.69406	-0.26721	0.37238
C	-2.23579	-0.09508	-0.02163	N	2.41712	0.55224	0.10779
C	-2.96110	-0.68348	-1.07732	C	5.16416	1.04857	0.50227
C	-2.87029	0.54886	1.05486	H	5.36605	-1.12858	0.41608
C	-4.36748	-0.73754	-0.97773	C	2.88179	1.81721	0.22807
H	-2.46127	-1.08835	-1.96763	C	4.24229	2.10024	0.42652
C	-4.27541	0.49594	1.12661	H	6.22975	1.24419	0.65546
H	-2.29570	1.03248	1.85350	H	2.12864	2.60648	0.16683
C	-5.01591	-0.14452	0.11668	H	4.55973	3.14308	0.51631
H	-4.94550	-1.20910	-1.77984	Pd	0.45480	-0.02749	-0.24257
H	-4.78696	0.95116	1.98186	C	-3.68747	-1.23313	-0.76004
H	-6.10930	-0.16208	0.17411	C	-2.48586	-0.75375	-0.11051
O	3.80498	-0.66607	0.11105	C	-2.55759	-0.25811	1.31435
H	4.51153	-2.44267	-0.72324	C	-3.72847	-0.88950	2.08834
H	2.23765	-3.31408	-0.69793	C	-5.04414	-0.76703	1.30008
				C	-4.90826	-1.22023	-0.13578
12				H	-1.58124	-0.44119	1.80016
E(Solv):	-1201.899708			H	-3.58918	-1.55488	-1.80296
Correction to H:	0.416946			H	-3.51412	-1.96041	2.26636
Correction to G:	0.332190			H	-3.82753	-0.41264	3.07845
C	2.73419	-1.80938	-0.00415	H	-5.85330	-1.33645	1.79424
C	2.60438	-4.04598	-0.22806	H	-5.39228	0.28899	1.29052
C	1.19543	-3.39687	-0.37668	H	-2.66651	0.84576	1.26228
N	1.45818	-1.95333	-0.20760	O	-1.40850	-0.73885	-0.78694
H	2.96344	-4.54783	-1.13940	C	-6.16091	-1.62558	-0.85501

H	-5.98215	-1.86750	-1.91462
H	-6.61845	-2.50544	-0.36180
H	-6.91711	-0.81870	-0.79815
C	-0.27727	1.83366	-0.25812
C	-0.78100	2.35551	-1.46684
C	-0.30473	2.62946	0.90777
C	-1.29164	3.66728	-1.51068
H	-0.77678	1.74771	-2.37935
C	-0.82593	3.93814	0.85754
H	0.07444	2.23979	1.86109
C	-1.31618	4.45882	-0.35082
H	-1.67009	4.06716	-2.45858
H	-0.84715	4.54614	1.76965
O	3.51218	-2.90489	0.02086
H	0.48302	-3.73861	0.39397
H	2.69751	-4.72436	0.63341
H	0.74086	-3.57670	-1.36584
H	-1.71609	5.47781	-0.38832

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E(Solv): -1201.878758

Correction to H: 0.416569

Correction to G: 0.334485

C	2.93201	-0.76633	0.13443
C	3.80122	-2.82238	0.42248
C	2.25037	-2.88939	0.33768
N	1.85320	-1.49046	0.04810
H	4.22108	-3.21273	1.36060
H	1.78439	-3.21022	1.28693
C	2.90179	0.69712	0.00010
C	4.06133	1.48120	0.01904
N	1.64794	1.22976	-0.13633
C	3.93453	2.87295	-0.11169
H	5.03488	0.99753	0.13480
C	1.53600	2.56996	-0.26270
C	2.65408	3.42036	-0.25652
H	4.82181	3.51331	-0.10020
H	0.51926	2.95559	-0.37094
H	2.50424	4.49866	-0.36188
Pd	0.05053	-0.21690	-0.09772
C	-1.27743	-1.92128	0.23212
C	-2.29561	-1.66806	1.31994
C	-3.68433	-1.20928	0.88431
C	-4.02438	-1.63241	-0.55578
C	-2.92443	-1.19193	-1.54933
C	-1.56485	-1.73046	-1.13562
H	-4.40965	-1.60032	1.61847
H	-0.50207	-2.64068	0.52996
H	-4.14102	-2.73223	-0.60466
H	-4.99111	-1.19738	-0.86315
H	-3.15150	-1.55192	-2.56933
H	-2.90518	-0.08795	-1.60832

H	-3.70694	-0.10442	0.97072	C	3.96405	-2.30415	-0.49622
O	-1.98924	-1.86802	2.49430	C	2.44981	-2.48258	-0.77399
C	-1.29775	1.25234	0.02765	N	1.87637	-1.17888	-0.35968
C	-1.72379	1.97189	-1.10704	H	4.31033	-2.81725	0.41570
C	-1.69223	1.66477	1.31513	H	1.98877	-3.30552	-0.20809
C	-2.55831	3.09814	-0.94880	C	2.66189	1.04460	0.18887
H	-1.40510	1.67621	-2.11460	C	3.70510	1.94541	0.43573
C	-2.52745	2.79102	1.46131	N	1.34361	1.40500	0.21339
H	-1.37054	1.11327	2.20677	C	3.37996	3.28233	0.71409
C	-2.96143	3.50604	0.33273	H	4.74062	1.59606	0.40458
H	-2.88837	3.65237	-1.83495	C	1.04274	2.69187	0.47950
H	-2.83731	3.10190	2.46548	C	2.03069	3.65866	0.73347
H	-3.61122	4.37933	0.45208	H	4.16929	4.01447	0.91027
C	-0.74589	-2.37520	-2.22682	H	-0.02128	2.94285	0.48993
H	0.24827	-2.70289	-1.88683	H	1.73184	4.68993	0.94217
H	-1.29817	-3.26200	-2.60044	Pd	-0.02389	-0.25131	-0.20799
H	-0.62402	-1.69856	-3.09165	C	-1.30973	-1.83687	-0.64916
O	4.10185	-1.37604	0.38044	C	-0.87146	-2.97155	0.24244
H	4.31264	-3.28173	-0.43816	C	-1.39883	-3.01925	1.67361
H	1.90173	-3.56478	-0.46161	C	-2.09506	-1.72094	2.10799
				C	-3.11492	-1.29144	1.04476

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E(Solv): -1201.870508

Correction to H: 0.415421

Correction to G: 0.337008

C	2.87588	-0.36967	-0.14044	C	-2.50384	-1.06298	-0.33402
				H	-1.12949	-2.05367	-1.71598
				O	-0.14536	-3.86069	-0.21191
				C	-3.52105	-0.86126	-1.44598
				H	-3.05048	-0.65773	-2.41995

H	-4.08664	-1.80952	-1.54591
H	-4.23850	-0.05902	-1.21108
C	-1.74521	0.92955	-0.23805
C	-1.85071	1.60209	-1.48424
C	-2.18149	1.59910	0.93233
C	-2.35116	2.91155	-1.55256
H	-1.53676	1.10199	-2.40788
C	-2.70847	2.89993	0.85701
H	-2.10723	1.11278	1.91066
C	-2.79428	3.55763	-0.38363
H	-2.41350	3.41973	-2.52104
H	-3.05167	3.39898	1.77015
H	-3.21364	4.56776	-0.44093
O	4.12186	-0.85032	-0.25181
H	4.61657	-2.56158	-1.34238
H	-1.33530	-0.92424	2.24737
H	-2.59556	-1.86087	3.08211
H	-3.71081	-0.41696	1.35385
H	-3.84819	-2.11566	0.90350
H	-2.11200	-3.86770	1.71446
H	-0.56484	-3.29635	2.34287
H	2.22197	-2.64545	-1.84237

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E(Solv): -1201.896346

Correction to H: 0.418234

Correction to G: 0.339449

C	-3.29596	0.48095	-0.00679
C	-5.21714	-0.63841	0.35089
C	-3.99960	-1.59842	0.51254
N	-2.84979	-0.72294	0.20995
H	-5.81837	-0.51703	1.26364
H	-3.89769	-2.00193	1.53437
C	-2.35330	1.55889	-0.31141
C	-2.74009	2.86616	-0.61940
N	-1.03894	1.15179	-0.28418
C	-1.74417	3.80729	-0.92614
H	-3.80258	3.12488	-0.61983
C	-0.08982	2.06425	-0.58720
C	-0.40715	3.39397	-0.91452
H	-2.01300	4.83911	-1.17166
H	0.94460	1.71602	-0.56155
H	0.40823	4.08363	-1.14809
Pd	-0.77440	-0.87049	0.19965
C	1.35652	-1.43276	0.63139
C	0.70579	-2.57488	0.05345
C	1.20718	-3.31345	-1.16500
C	2.65063	-2.92693	-1.54494
C	2.91388	-1.42207	-1.34799
C	2.71949	-0.95351	0.12215
H	1.10718	-4.39626	-0.96119
H	1.15261	-1.28025	1.70292

H	3.36652	-3.51726	-0.94591
H	2.83626	-3.20066	-2.59796
H	3.94598	-1.19512	-1.66938
H	2.23749	-0.84415	-2.00970
H	0.50394	-3.10310	-1.99437
O	-0.47704	-2.85669	0.55059
C	3.79139	-1.63400	1.03927
H	3.71012	-2.73412	1.02226
H	4.80290	-1.35036	0.69844
H	3.68487	-1.30589	2.08678
C	2.89400	0.57147	0.29315
C	2.57912	1.18474	1.52879
C	3.42246	1.38848	-0.72950
C	2.76853	2.55969	1.73051
H	2.18469	0.58368	2.35608
C	3.61786	2.76814	-0.52911
H	3.69414	0.95810	-1.69758
C	3.28947	3.36064	0.69924
H	2.51957	3.00384	2.70053
H	4.04164	3.37387	-1.33788
H	3.45248	4.43179	0.85961
O	-4.61571	0.68703	0.05461
H	-5.86935	-0.88632	-0.50005
H	-4.02121	-2.44619	-0.19192

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E(Solv): -1201.860068

Correction to H: 0.415180

Correction to G: 0.335450

C	2.95586	-0.61777	0.09199
C	3.93445	-2.64385	0.18029
C	2.42498	-2.78227	-0.16184
N	1.92088	-1.39135	-0.09244
H	4.20109	-3.03356	1.17545
H	2.25645	-3.18179	-1.17720
C	2.82930	0.84319	0.15872
C	3.91796	1.70424	0.34602
N	1.54562	1.28213	0.01422
C	3.67221	3.08618	0.38211
H	4.92494	1.29320	0.45730
C	1.31992	2.60956	0.05173
C	2.35630	3.54265	0.23194
H	4.49725	3.79083	0.52471
H	0.27948	2.92365	-0.06998
H	2.12073	4.61060	0.25228
Pd	0.06176	-0.34875	-0.25472
C	-1.24215	-1.99834	-0.55681
C	-1.36431	-2.85049	0.70829
C	-1.99091	-2.09345	1.89113
C	-3.37575	-1.53710	1.51396
C	-3.43453	-0.85864	0.14726
C	-2.17008	-0.89072	-0.71908

H	-4.11881	-2.35831	1.47079
H	-3.76605	-0.83131	2.26952
C	-1.54350	0.99010	-0.25845
C	-1.75567	1.80089	-1.39955
C	-1.87173	1.49816	1.02357
C	-2.24527	3.10920	-1.25421
H	-1.54340	1.41168	-2.40160
C	-2.35750	2.80953	1.15707
H	-1.74036	0.88120	1.91874
C	-2.55062	3.61592	0.02155
H	-2.40411	3.72599	-2.14556
H	-2.59948	3.19420	2.15395
H	-2.95296	4.62851	0.12879
H	-1.31072	-1.27418	2.19627
H	-2.08417	-2.76321	2.76397
H	-2.40715	-0.61932	-1.75570
C	-0.83404	-2.75349	-1.81627
H	0.06123	-3.37565	-1.64946
H	-1.65077	-3.44138	-2.11497
H	-0.63963	-2.07798	-2.66658
H	-1.99310	-3.73270	0.45580
H	-0.37666	-3.26247	0.98638
O	-4.46529	-0.40402	-0.32872
H	4.61080	-3.06222	-0.57899
H	1.88548	-3.42253	0.55568
O	4.16454	-1.18565	0.21354

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E(Solv): -1201.885711

Correction to H: 0.417152

Correction to G: 0.336879

C	-2.70572	-1.30219	-0.11775
C	-2.96440	-3.53796	-0.16221
C	-1.45892	-3.16553	-0.19446
N	-1.46328	-1.69359	-0.02001
H	-3.29854	-4.15584	-1.00770
H	-0.98056	-3.41540	-1.15862
C	-3.09052	0.11345	-0.07938
C	-4.42802	0.53347	-0.07253
N	-2.03073	0.97160	-0.03653
C	-4.69187	1.90999	-0.00322
H	-5.23179	-0.20649	-0.11455
C	-2.30094	2.28889	0.03738
C	-3.61121	2.79918	0.05898
H	-5.72287	2.27682	0.00642
H	-1.43103	2.95031	0.07260
H	-3.76846	3.88001	0.12103
Pd	-0.02420	-0.13867	0.10337
C	1.65899	-1.25440	0.64221
C	2.08120	-2.35206	-0.35666
C	3.13759	-1.94143	-1.39690
C	4.36316	-1.30707	-0.71075

C	3.98245	-0.04811	0.04849	H	-0.88585	-3.65171	0.61091
C	2.60542	-0.04405	0.78419	O	-3.65549	-2.23832	-0.26968
H	4.78331	-2.02977	0.02088				
H	5.17242	-1.05547	-1.41637	**18**			
C	1.79355	1.18463	0.33137	E(Solv):	-1278.314466		
C	1.60285	2.30464	1.19884	Correction to H:	0.444488		
C	1.44126	1.32835	-1.05210	Correction to G:	0.359106		
C	1.14784	3.52343	0.69856	C	-3.80028	-0.46811	0.44023
H	1.88215	2.21155	2.25416	C	-4.56608	-2.48813	1.08140
C	0.96049	2.57043	-1.54061	C	-3.05328	-2.59299	0.72009
H	1.73688	0.56279	-1.77834	N	-2.73710	-1.21639	0.29533
C	0.83794	3.66129	-0.67738	H	-4.79515	-2.73581	2.12778
H	1.05860	4.38608	1.36740	H	-2.84848	-3.29424	-0.10489
H	0.74136	2.67897	-2.60793	C	-3.71840	0.95485	0.10719
H	0.52012	4.63451	-1.06776	C	-4.75898	1.88023	0.23149
H	2.71327	-1.24018	-2.14158	N	-2.46507	1.30680	-0.33719
H	3.45281	-2.83231	-1.96873	C	-4.50620	3.21967	-0.10647
H	2.85457	0.10313	1.85354	H	-5.73792	1.54861	0.58899
C	1.26757	-1.83563	2.00578	C	-2.22544	2.59905	-0.65090
H	0.52879	-2.65094	1.91993	C	-3.22427	3.58004	-0.54877
H	2.16699	-2.26457	2.49756	H	-5.29831	3.96938	-0.02079
H	0.85619	-1.07100	2.68931	H	-1.20889	2.82987	-0.98137
H	2.50973	-3.18555	0.24290	H	-2.98612	4.61366	-0.81524
H	1.19810	-2.78272	-0.86169	Pd	-1.12679	-0.26339	-0.43059
O	4.68403	0.95206	0.10325	C	1.96800	-0.96315	0.41445
H	-3.28529	-3.99544	0.78773	C	1.29402	-1.88078	-0.36097

C	2.00946	-2.92025	-1.20485	H	4.93741	4.44070	0.42240
C	3.48039	-3.07361	-0.77897	O	0.48483	0.84993	-1.23980
C	4.13977	-1.69571	-0.60741	H	1.27289	0.34606	-0.81519
C	3.49029	-0.85889	0.52998	H	0.54803	0.66113	-2.20461
H	1.45755	-3.87411	-1.11493	H	-5.22482	-3.05338	0.40536
H	1.36960	-0.36018	1.11536	H	-2.41714	-2.86993	1.57701
H	3.53541	-3.64789	0.16421	O	-4.90855	-1.05015	0.89989
H	4.02520	-3.66412	-1.53699				
H	5.22153	-1.80890	-0.41124	**19-ts**			
H	4.04510	-1.14805	-1.56622	E(Solv):	-1278.309627		
H	1.93658	-2.63078	-2.27352	Correction to H:	0.440132		
O	-0.04805	-1.94364	-0.47030	Correction to G:	0.357169		
C	3.93806	-1.41509	1.91650	C	-3.84684	-0.40205	0.39138
H	3.68633	-2.48510	2.01767	C	-4.72185	-2.38482	1.00750
H	5.02872	-1.29392	2.04299	C	-3.21309	-2.56158	0.65714
H	3.44271	-0.87657	2.74271	N	-2.80871	-1.19106	0.28768
C	3.90205	0.63571	0.46362	H	-5.40301	-2.93834	0.34481
C	3.30880	1.56933	1.34610	H	-3.03915	-3.24095	-0.19359
C	4.88809	1.11550	-0.42406	C	-3.69252	1.02131	0.07915
C	3.67195	2.92383	1.33248	C	-4.69023	1.99428	0.18213
H	2.56105	1.23547	2.07604	N	-2.41278	1.32131	-0.32095
C	5.25557	2.47257	-0.44089	C	-4.36101	3.32351	-0.13349
H	5.39694	0.43014	-1.10827	H	-5.69505	1.70798	0.50517
C	4.64751	3.38451	0.43285	C	-2.09466	2.60093	-0.61018
H	3.19881	3.61884	2.03559	C	-3.05042	3.62706	-0.52973
H	6.02880	2.81168	-1.13930	H	-5.11880	4.10963	-0.06443

H	-1.05416	2.77409	-0.90051	C	5.40432	2.36414	-0.45897
H	-2.75545	4.65083	-0.77672	H	5.48472	0.30037	-1.06747
Pd	-1.14024	-0.27974	-0.39037	C	4.79177	3.32694	0.35504
C	1.91083	-0.89292	0.31579	H	3.26503	3.67368	1.86191
C	1.24875	-1.94555	-0.34628	H	6.22727	2.64893	-1.12400
C	1.98831	-3.03264	-1.09831	H	5.12923	4.36872	0.33176
C	3.46178	-3.14207	-0.66989	O	0.47893	0.81021	-1.06496
C	4.10593	-1.74986	-0.57013	H	1.35510	0.10544	-0.57402
C	3.44024	-0.85269	0.50935	H	0.54566	0.68537	-2.04064
H	1.43753	-3.98132	-0.95949	H	-4.96335	-2.59553	2.05961
H	1.31793	-0.43200	1.12677	H	-2.60748	-2.91040	1.50975
H	3.53104	-3.67149	0.29778	O	-5.00030	-0.93881	0.78990
H	4.00897	-3.76190	-1.40210				
H	5.18434	-1.84947	-0.35052	**20**			
H	4.02649	-1.25484	-1.55866	E(Solv):	-1278.329982		
H	1.91002	-2.80131	-2.18098	Correction to H:	0.445383		
O	-0.06059	-1.99208	-0.49508	Correction to G:	0.358210		
C	3.79792	-1.38282	1.92907	C	-3.26638	-0.52105	1.16698
H	3.47026	-2.42847	2.06709	C	-3.28017	-2.28583	2.56504
H	4.88834	-1.33077	2.09698	C	-2.11714	-2.42622	1.53775
H	3.31195	-0.77683	2.71334	N	-2.22133	-1.18483	0.74328
C	3.92308	0.61681	0.41917	H	-4.02681	-3.09142	2.51082
C	3.32296	1.60087	1.23867	H	-2.23097	-3.29896	0.87194
C	4.97515	1.02563	-0.42603	C	-3.63621	0.73511	0.51308
C	3.74686	2.93700	1.20891	C	-4.71116	1.55841	0.86287
H	2.51610	1.32127	1.92757	N	-2.79763	1.04013	-0.52777

C	-4.92193	2.73048	0.11743	H	3.15570	-1.16729	2.43678
H	-5.35953	1.27869	1.69782	H	1.75471	-0.16591	1.98597
C	-2.99553	2.16359	-1.24545	C	3.91221	0.75657	0.56863
C	-4.05423	3.03548	-0.94203	C	3.19540	1.92127	0.92703
H	-5.75497	3.39577	0.36395	C	5.31464	0.85623	0.45971
H	-2.27576	2.31269	-2.05921	C	3.85061	3.13827	1.15979
H	-4.18771	3.94063	-1.54119	H	2.10375	1.88618	1.02829
Pd	-1.29316	-0.28454	-0.86802	C	5.97514	2.07401	0.69686
C	2.08261	-0.30942	-0.81088	H	5.91704	-0.01718	0.19409
C	1.38777	-1.57323	-1.22259	C	5.24778	3.22043	1.04482
C	2.25086	-2.74379	-1.60814	H	3.26725	4.02453	1.43280
C	3.33871	-3.00151	-0.52902	H	7.06600	2.11982	0.60795
C	4.08445	-1.71102	-0.14744	H	5.76326	4.16931	1.22687
C	3.15106	-0.56480	0.32834	O	-0.65492	0.83393	-2.35850
H	1.62525	-3.63033	-1.80155	H	2.62290	0.08044	-1.69644
H	1.33623	0.44864	-0.52348	H	-0.50113	0.23010	-3.11960
H	2.86819	-3.46213	0.35841	O	-3.97208	-1.03201	2.18177
H	4.05150	-3.74654	-0.92342	H	-2.94147	-2.15618	3.60421
H	4.81696	-1.94105	0.64769	H	-1.12683	-2.48302	2.01929
H	4.66632	-1.36394	-1.02366				
H	2.75580	-2.46825	-2.55754				
O	0.13430	-1.72692	-1.23489				
C	2.42241	-0.97134	1.63529				
H	1.80859	-1.88275	1.50398				